

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'HOME' AT 07:10:27 ON 27 JUN 2003
FILE 'HOME' ENTERED AT 07:10:27 ON 27 JUN 2003

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.05	1.05

=> FIL STNGUIDE	SINCE FILE ENTRY	TOTAL SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	1.05	1.05

FILE 'STNGUIDE' ENTERED AT 07:10:37 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 20, 2003 (20030620/UP).

=> FIL HOME	SINCE FILE ENTRY	TOTAL SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	0.06	1.11

FILE 'HOME' ENTERED AT 07:10:40 ON 27 JUN 2003

=> FIL STNGUIDE	SINCE FILE ENTRY	TOTAL SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	0.21	1.32

FILE 'STNGUIDE' ENTERED AT 07:10:52 ON 27 JUN 2003
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 20, 2003 (20030620/UP).

=> FIL HOME	SINCE FILE ENTRY	TOTAL SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	0.12	1.44

FILE 'HOME' ENTERED AT 07:12:21 ON 27 JUN 2003

=> FIL STNGUIDE	SINCE FILE ENTRY	TOTAL SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	0.21	1.65

FILE 'STNGUIDE' ENTERED AT 07:12:34 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jun 20, 2003 (20030620/UP).

=> FIL HOME	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.06	1.71

FILE 'HOME' ENTERED AT 07:13:22 ON 27 JUN 2003

=> logoff hold	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.84	2.55

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:15:28 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTA1623PAZ

PASSWORD:
LOGINID/PASSWORD REJECTED

The loginid and/or password sent to STN were invalid.
You either typed them incorrectly, or line noise may
have corrupted them.

Do you wish to retry the logon?
Enter choice (y/N):

Connecting via Winsock to STN

LOGINID:

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTA1623PAZ

PASSWORD:
LOGINID/PASSWORD REJECTED

The loginid and/or password sent to STN were invalid.
You either typed them incorrectly, or line noise may
have corrupted them.

Do you wish to retry the logon?
Enter choice (y/N):

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?): 2

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 Jun 03 New e-mail delivery for search results now available
NEWS 4 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN
NEWS 6 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 7 Sep 03 JAPIO has been reloaded and enhanced
NEWS 8 Sep 16 Experimental properties added to the REGISTRY file
NEWS 9 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 10 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11 Oct 24 BEILSTEIN adds new search fields
NEWS 12 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13 Nov 18 DKILIT has been renamed APOLLIT
NEWS 14 Nov 25 More calculated properties added to REGISTRY
NEWS 15 Dec 04 CSA files on STN
NEWS 16 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17 Dec 17 TOXCENTER enhanced with additional content
NEWS 18 Dec 17 Adis Clinical Trials Insight now available on STN
NEWS 19 Jan 29 Simultaneous left and right truncation added to COMPENDEX,
ENERGY, INSPEC
NEWS 20 Feb 13 CANCERLIT is no longer being updated
NEWS 21 Feb 24 METADEX enhancements
NEWS 22 Feb 24 PCTGEN now available on STN
NEWS 23 Feb 24 TEMA now available on STN
NEWS 24 Feb 26 NTIS now allows simultaneous left and right truncation
NEWS 25 Feb 26 PCTFULL now contains images
NEWS 26 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27 Mar 20 EVENTLINE will be removed from STN
NEWS 28 Mar 24 PATDPAFULL now available on STN
NEWS 29 Mar 24 Additional information for trade-named substances without
structures available in REGISTRY
NEWS 30 Apr 11 Display formats in DGENE enhanced
NEWS 31 Apr 14 MEDLINE Reload
NEWS 32 Apr 17 Polymer searching in REGISTRY enhanced
NEWS 33 Jun 13 Indexing from 1947 to 1956 added to records in CA/CAPLUS
NEWS 34 Apr 21 New current-awareness alert (SDI) frequency in
WPIDS/WPINDEX/WPIX
NEWS 35 Apr 28 RDISCLOSURE now available on STN
NEWS 36 May 05 Pharmacokinetic information and systematic chemical names
added to PHAR
NEWS 37 May 15 MEDLINE file segment of TOXCENTER reloaded
NEWS 38 May 15 Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39 May 16 CHEMREACT will be removed from STN
NEWS 40 May 19 Simultaneous left and right truncation added to WSCA
NEWS 41 May 19 RAPRA enhanced with new search field, simultaneous left and
right truncation
NEWS 42 Jun 06 Simultaneous left and right truncation added to CBNB
NEWS 43 Jun 06 PASCAL enhanced with additional data
NEWS 44 Jun 20 2003 edition of the FSTA Thesaurus is now available
NEWS 45 Jun 25 HSDB has been reloaded

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 08:29:25 ON 27 JUN 2003

=> logoff hold
COST IN U.S. DOLLARS
SINCE FILE ENTRY 0.84
TOTAL SESSION 0.84
FULL ESTIMATED COST

SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 08:31:42 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'HOME' AT 08:44:40 ON 27 JUN 2003
FILE 'HOME' ENTERED AT 08:44:40 ON 27 JUN 2003

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.84	0.84

=> file mreg
'MREG' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'HOME'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files
that are available. If you have requested multiple files, you can
specify a corrected file name or you can enter "IGNORE" to continue
accessing the remaining file names entered.

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.05	1.05

FILE 'REGISTRY' ENTERED AT 08:45:01 ON 27 JUN 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See **HELP CROSSOVER** for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
Uploading 10075845 generic six.str

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

```
=> search 11 sss sam
SAMPLE SEARCH INITIATED 08:45:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE
```

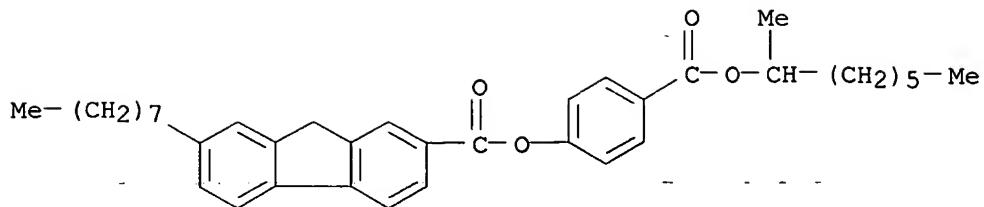
32.4% PROCESSED 1000 ITERATIONS 3 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00:00:01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTION ITERATIONS: 58448 TO 65112
PROJECTION ANSWERS: 3 TO 367

L2 3 SEA SSS SAM L1

=> d scan

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-octyl-, 4-[[[(1-
methylheptyl)oxy]carbonyl]phenyl ester (9CI)
MF C37 H46 O4



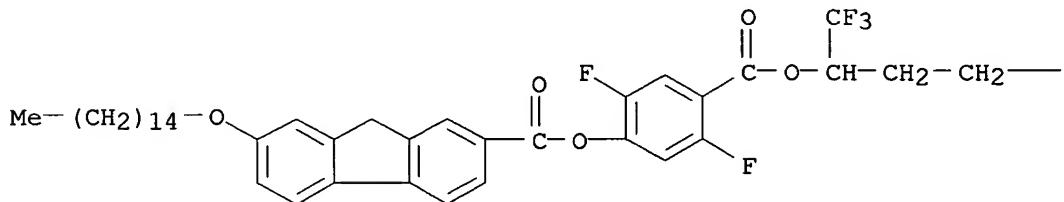
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
 'LOFGOFF HOLD' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".
 HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(pentadecyloxy)-, 4-[[[4-ethyl-1-(trifluoromethyl)hexyl]oxy]carbonyl]-2,5-difluorophenyl ester (9CI)
 MF C45 H57 F5 O5

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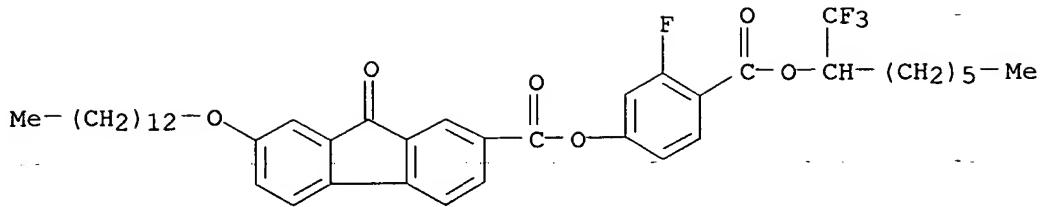


PAGE 1-B

— CH₂Et₂

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 9-oxo-7-(tridecyloxy)-,
 3-fluoro-4-[[[1-(trifluoromethyl)heptyl]oxy]carbonyl]phenyl ester (9CI)
 MF C42 H50 F4 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold			
COST IN U.S. DOLLARS	SINCE FILE	TOTAL	
	ENTRY	SESSION	
FULL ESTIMATED COST	0.80	1.85	

SESSION WILL BE HELD FOR 60 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 08:46:27 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:
 * * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
 SESSION RESUMED IN FILE 'REGISTRY' AT 08:48:38 ON 27 JUN 2003
 FILE 'REGISTRY' ENTERED AT 08:48:38 ON 27 JUN 2003
 COPYRIGHT (C) 2003 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL	
	ENTRY	SESSION	
FULL ESTIMATED COST	0.80	1.85	

=>
 Uploading 10075845 generic six.str

L3 STRUCTURE UPLOADED

=> d 113
 L13 NOT FOUND
 The L-number entered has not been defined in this session, or it
 has been deleted. To see the L-numbers currently defined in this
 session, enter DISPLAY HISTORY at an arrow prompt (>).

=> d 13
 L3 HAS NO ANSWERS
 L3 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> search 13 sss sam

SAMPLE SEARCH INITIATED 08:49:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.4% PROCESSED 1000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTED ITERATIONS: 58448 TO 65112
PROJECTED ANSWERS: 0 TO 0
BATCH **COMPLETE**

T4 0 SEA SSS SAM L3

```
=> search 13 sss full
FULL SEARCH INITIATED 08:50:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 62195 TO ITERATE
```

100.0% PROCESSED 62195 ITERATIONS
SEARCH TIME: 00.00.03

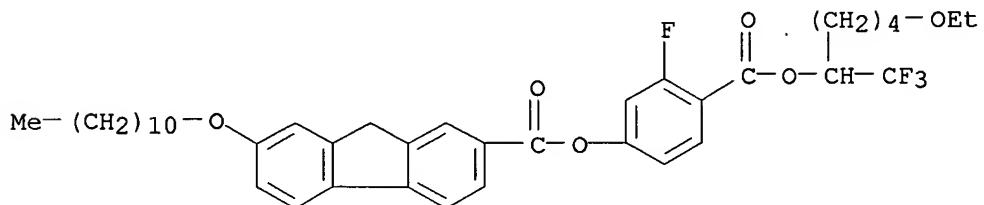
137 ANSWERS

L5 137 SEA SSS FUL L3

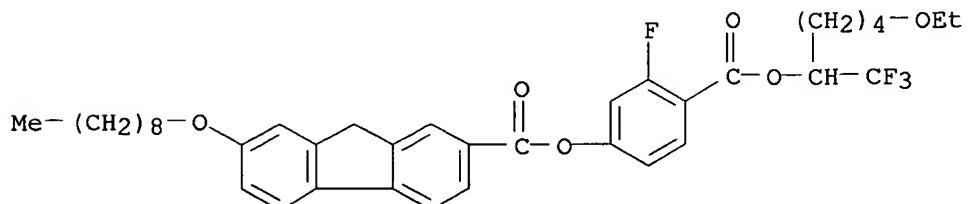
=> d scan

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl 7-(undecyloxy)-9H-fluorene-2-carboxylate, 1-methylheptyl 4-[6-(4-hexylphenyl)-3-pyridinyl]benzoate, 4-[[{(1-methylheptyl)oxy]carbonyl}phenyl 4'-(octyloxy)[1,1'-biphenyl]-4-carboxylate and 4-[[{(1-methylheptyl)oxy]carbonyl}phenyl 4-[[4-(undecyloxy)benzoyl]oxy]benzoate (9CI)
 MF C40 H52 O7 . C40 H48 F4 O6 . C38 H44 F4 O6 . C36 H46 O5 . C32 H41 N O2 .
 CI MXS

CM 1

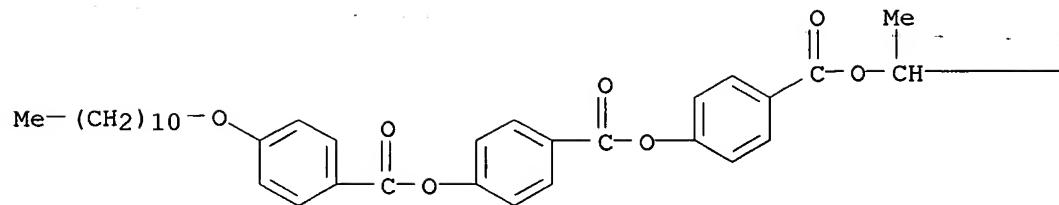


CM 2



CM 3

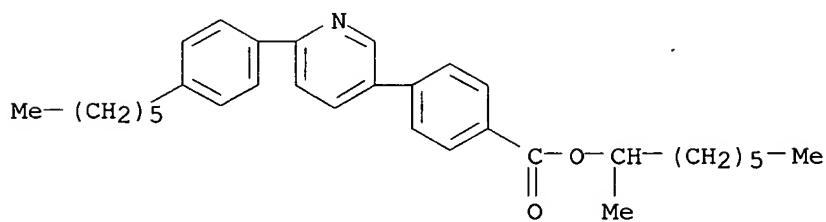
PAGE 1-A



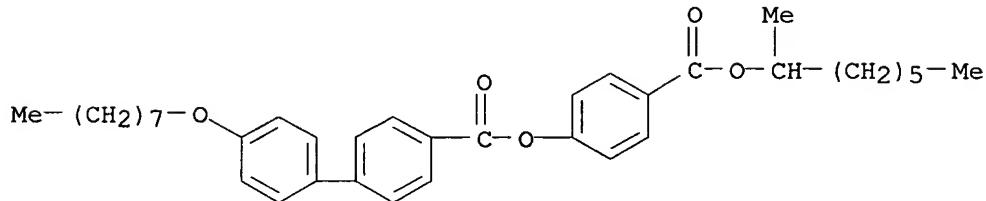
PAGE 1-B

— $(\text{CH}_2)_5-\text{Me}$

CM 4



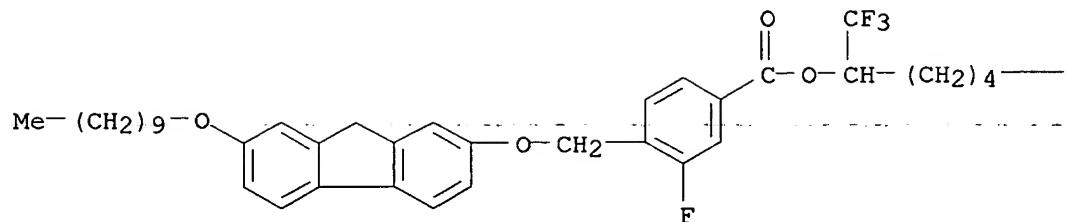
CM 5



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[[[7-(decyloxy)-9H-fluoren-2-yl]oxy]methyl]-3-fluoro-,
5-ethoxy-1-(trifluoromethyl)pentyl ester (9CI)
MF C39 H48 F4 O5

PAGE 1-A

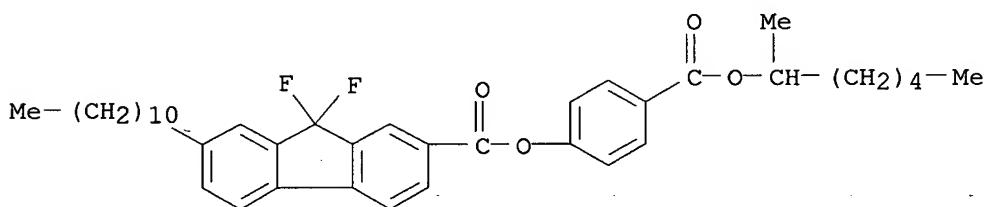


PAGE 1-B

—OEt

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

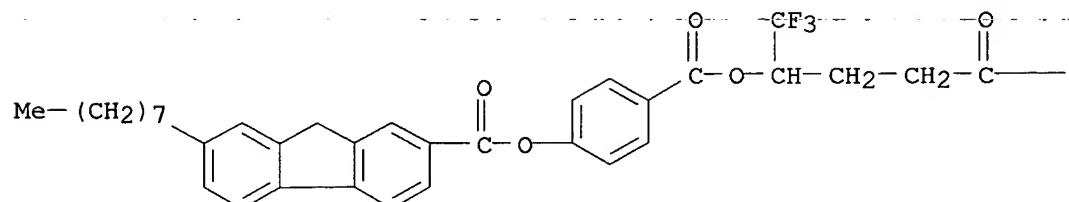
L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 9,9-difluoro-7-undecyl-,
4-[(1-methylhexyl)oxy]carbonylphenyl ester (9CI)
MF C39 H48 F2 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-octyl-, 4-[(4-butoxy-4-oxo-1-(trifluoromethyl)butoxy]carbonylphenyl ester (9CI)
MF C38 H43 F3 O6

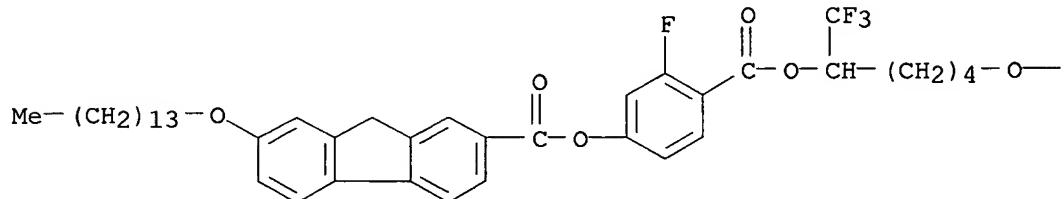
PAGE 1-A



— OBu-n

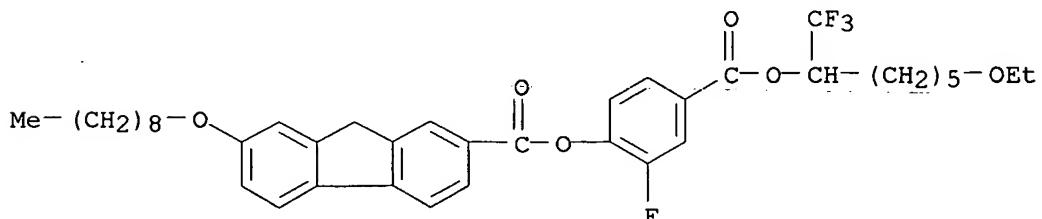
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(tetradecyloxy)-, 3-fluoro-4-[[2,2,2-trifluoro-1-[4-(2,2,2-trifluoroethoxy)butyl]ethoxy]carbonyl]phenyl ester (9CI)
 MF C43 H51 F7 O6

— CH₂—CF₃

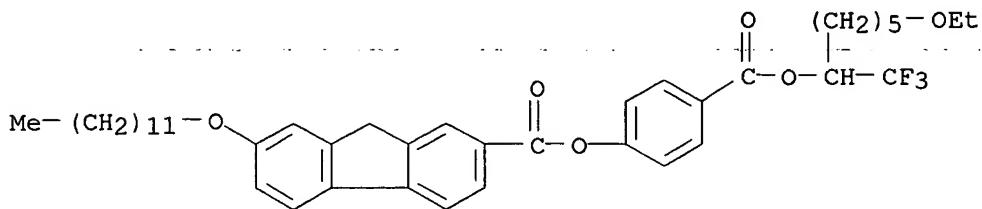
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[[6-ethoxy-1-(trifluoromethyl)hexyl]oxy]carbonyl]-2-fluorophenyl ester (9CI)
 MF C39 H46 F4 O6



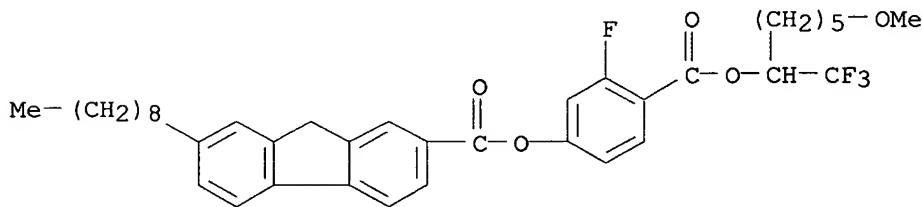
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[[6-ethoxy-1-(trifluoromethyl)hexyl]oxy]carbonyl]phenyl ester (9CI)
 MF C42 H53 F3 O6



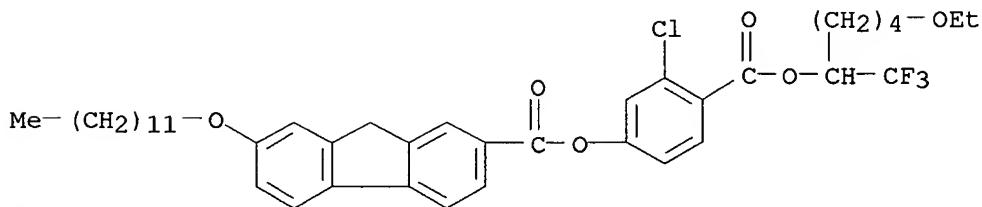
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-nonyl-, 3-fluoro-4-[[2,2,2-trifluoro-1-(5-methoxypentyl)ethoxy]carbonyl]phenyl ester (9CI)
 MF C38 H44 F4 O5



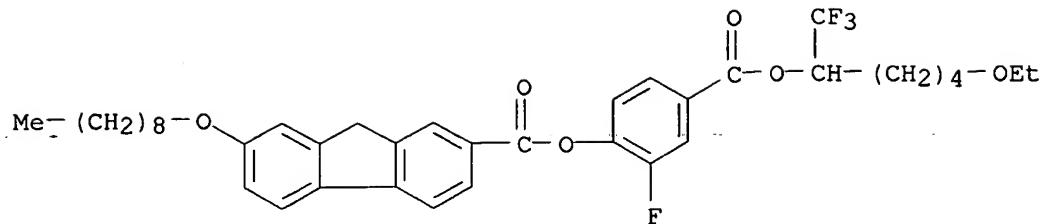
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 3-chloro-4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]phenyl ester (9CI)
 MF C41 H50 Cl F3 O6



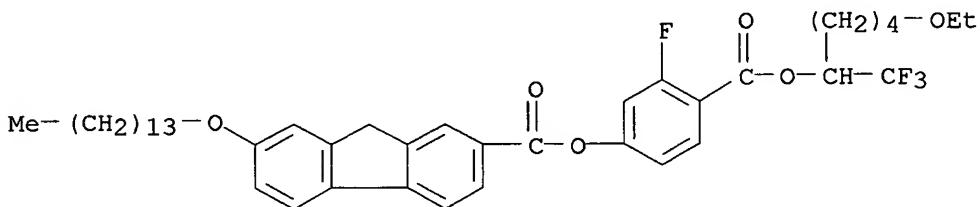
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-2-fluorophenyl ester (9CI)
 MF C38 H44 F4 O6



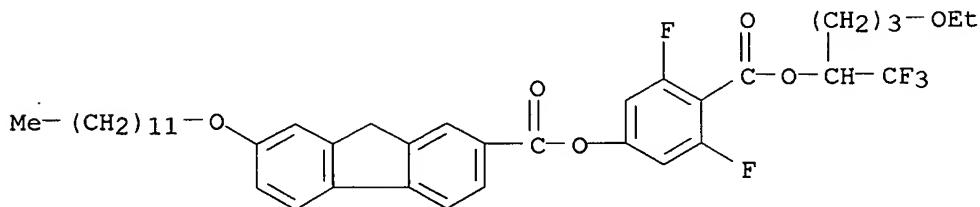
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(tetradecyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester (9CI)
 MF C43 H54 F4 O6



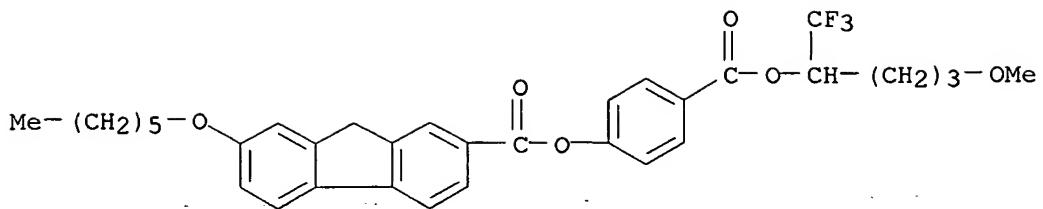
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[4-ethoxy-1-(trifluoromethyl)butoxy]carbonyl]-3,5-difluorophenyl ester (9CI)
 MF C40 H47 F5 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

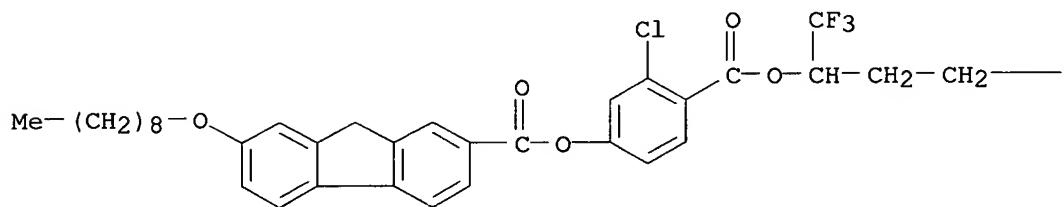
L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(hexyloxy)-, 4-[[4-methoxy-1-(trifluoromethyl)butoxy]carbonyl]phenyl ester (9CI)
 MF C33 H35 F3 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 3-chloro-4-[{3-ethoxy-1-(trifluoromethyl)propoxy}carbonyl]phenyl ester (9CI)
 MF C36 H40 Cl F3 O6

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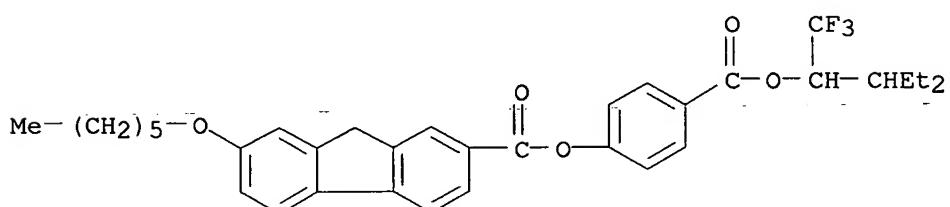


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—OEt

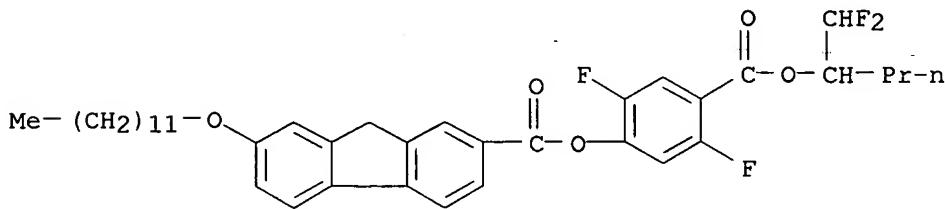
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN 9H-Fluorene-2-carboxylic acid, 7-(hexyloxy)-, 4-[{2-ethyl-1-(trifluoromethyl)butoxy}carbonyl]phenyl ester (9CI)
 MF C34 H37 F3 O5



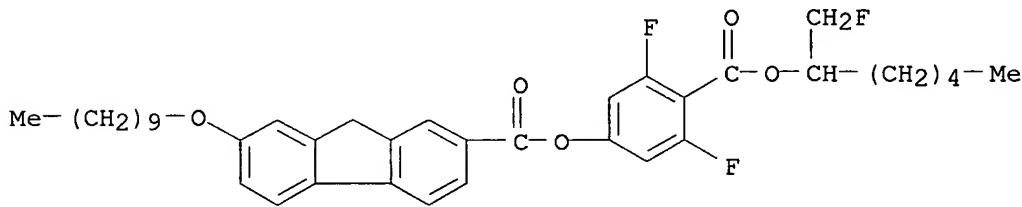
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[1-
(difluoromethyl)butoxy]carbonyl]-2,5-difluorophenyl ester (9CI)
MF C38 H44 F4 O5



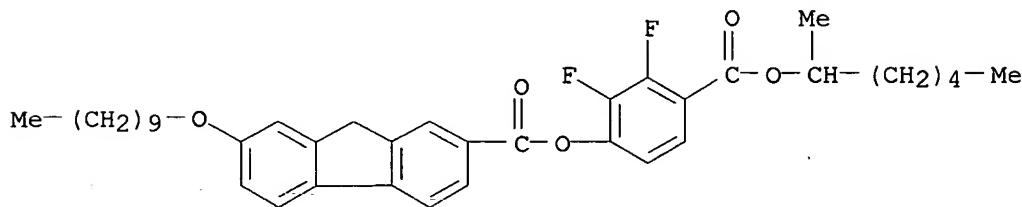
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(decyloxy)-, 3,5-difluoro-4-[[1-
(fluoromethyl)hexyl]oxy]carbonylphenyl ester (9CI)
MF C38 H45 F3 O5



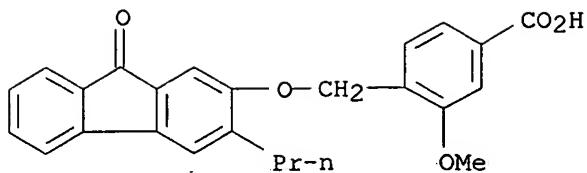
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(decyloxy)-, 2,3-difluoro-4-[[1-
(methylhexyl)oxy]carbonyl]phenyl ester (9CI)
MF C38 H46 F2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-methoxy-4-[[9-oxo-3-propyl-9H-fluoren-2-yl)oxy]methyl]-
(9CI)
MF C25 H22 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

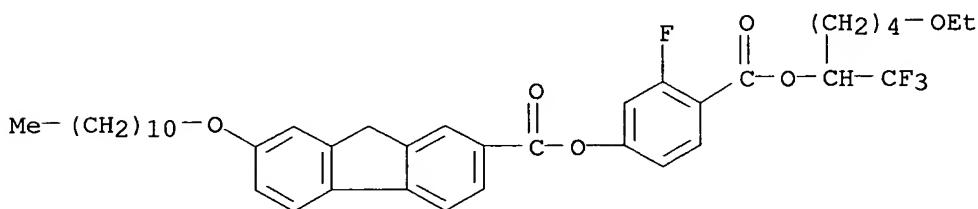
L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS.

IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl 7-(undecyloxy)-9H-fluorene-2-carboxylate, 4-[[1-(1-methylheptyl)oxy]carbonyl]phenyl 4-(octyloxy)benzoate, 4-[[1-(1-methylheptyl)oxy]carbonyl]phenyl 4'-(octyloxy)[1,1'-biphenyl]-4-carboxylate and 4-[[1-(1-methylheptyl)oxy]carbonyl]phenyl 4-[(4-(undecyloxy)benzoyl)oxy]benzoate (9CI)

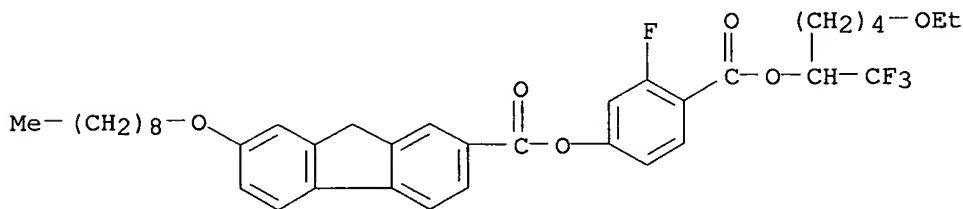
MF C40 H52 O7 . C40 H48 F4 O6 . C38 H44 F4 O6 . C36 H46 O5 . C30 H42 O5

CI MXS

CM 1

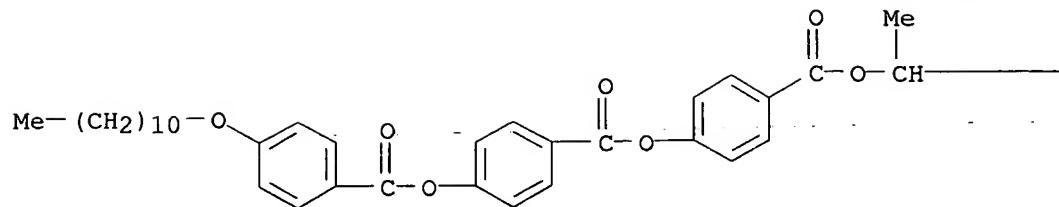


CM 2



CM 3

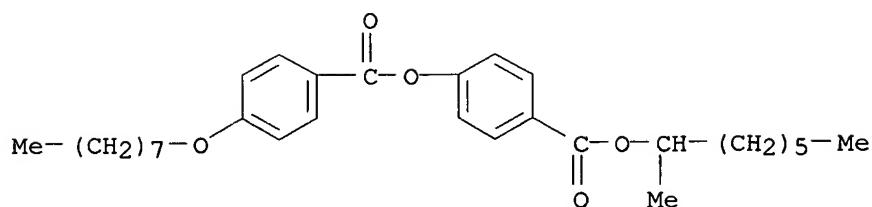
PAGE 1-A



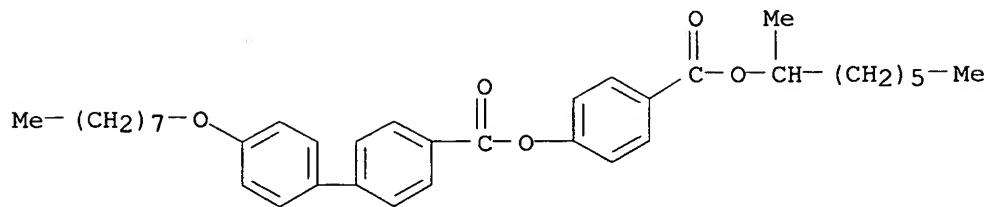
PAGE 1-B

$$-\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2-\text{Me}$$

CM 4

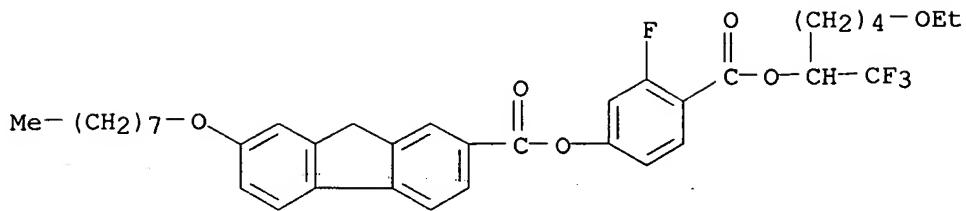


CM 5

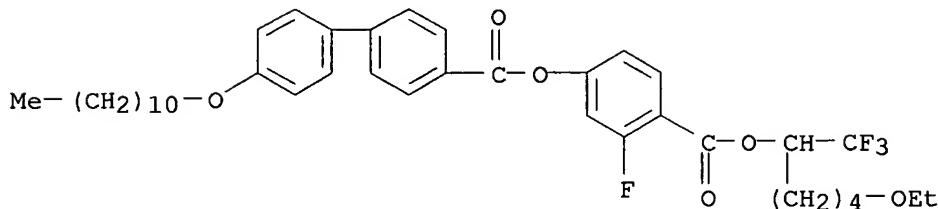


L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 9H-Fluorene-2-carboxylic acid, 7-(octyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with 4-[[[5-ethoxy-1-(trifluoromethyl)pentyl]oxy]carbonyl]-3-fluorophenyl 4'-(undecyloxy)[1,1'-biphenyl]-4-carboxylate (9CI)
MF C39 H48 F4 O6 . C37 H42 F4 O6
CI MXS

CM 1



CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=>
Uploading 10075845 generic six.str

L6 STRUCTURE UPLOADED

=> d 16
L6 HAS NO ANSWERS
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> search 16 sss sam
SAMPLE SEARCH INITIATED 08:54:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.4% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 58448 TO 65112
-PROJECTED- ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

=> search 16 sss full
FULL SEARCH INITIATED 08:54:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 62195 TO ITERATE

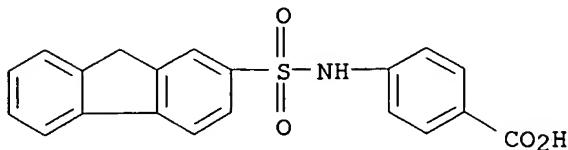
100.0% PROCESSED 62195 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.03

L8

3 SEA SSS FUL L6

=> d scan

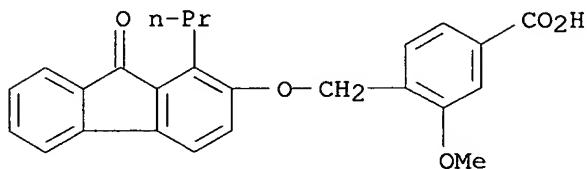
L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(9H-fluoren-2-ylsulfonyl)amino]- (9CI)
MF C20 H15 N O4 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

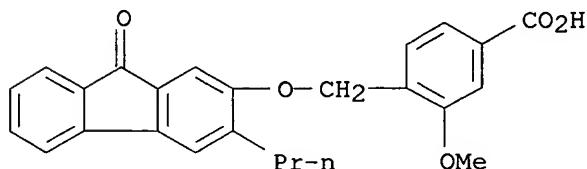
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-methoxy-4-[(9-oxo-1-propyl-9H-fluoren-2-yl)oxy]methyl- (9CI)
MF C25 H22 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 3-methoxy-4-[(9-oxo-3-propyl-9H-fluoren-2-yl)oxy]methyl- (9CI)
MF C25 H22 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	301.90	302.95

SESSION WILL BE HELD FOR 60 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 08:57:09 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
 SESSION RESUMED IN FILE 'REGISTRY' AT 09:05:09 ON 27 JUN 2003
 FILE 'REGISTRY' ENTERED AT 09:05:09 ON 27 JUN 2003
 COPYRIGHT (C) 2003 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	301.90	302.95

=>
 Uploading 10075845 generic six crrct.str

L9 STRUCTURE UPLOADED

=> d 19
 L9 HAS NO ANSWERS
 L9 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 Structure attributes must be viewed using STN Express query preparation.

=> search 19 sss sam
 SAMPLE SEARCH INITIATED 09:06:14 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 3229 TO ITERATE

31.0% PROCESSED 1000 ITERATIONS 0 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 61173 TO 67987
 PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

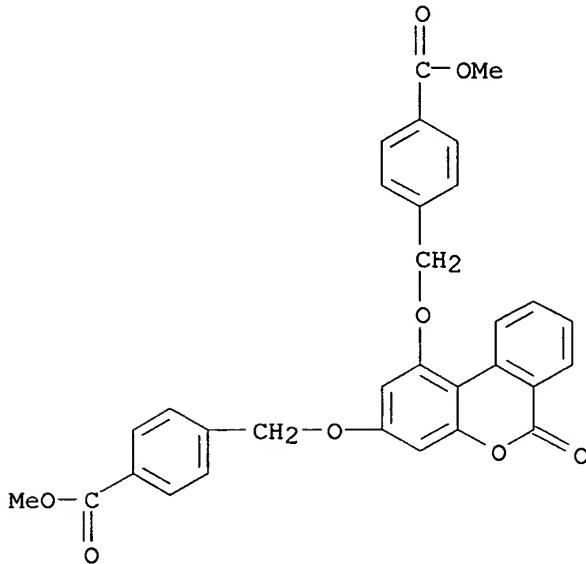
=> search 19 sss full
 FULL SEARCH INITIATED 09:06:24 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 65007 TO ITERATE

100.0% PROCESSED 65007 ITERATIONS 6 ANSWERS
 SEARCH TIME: 00.00.03

L11 6 SEA SSS FUL L9

=> d scan

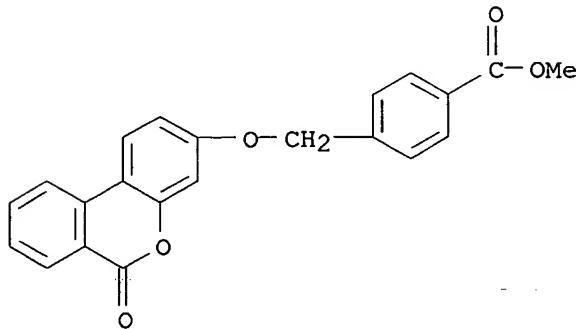
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4,4'-(6-oxo-6H-dibenzo[b,d]pyran-1,3-diyil)bis(oxymethylene)bis-, dimethyl ester (9CI)
MF C31 H24 O8



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):6

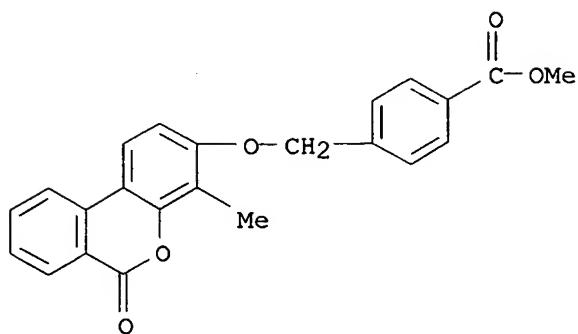
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester (9CI)
MF C22 H16 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

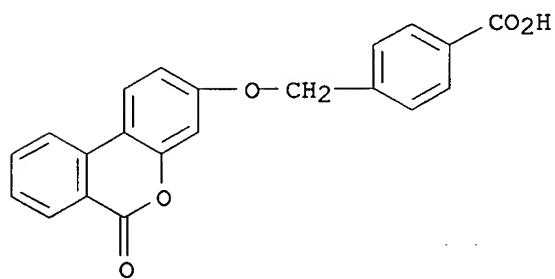
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-,

methyl ester (9CI)
MF C23 H18 O5



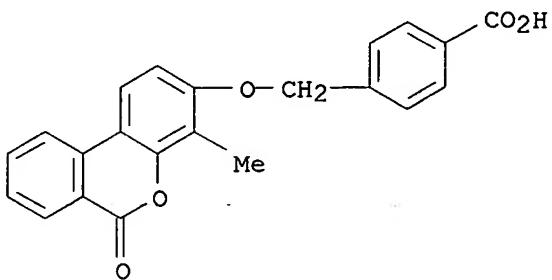
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl- (9CI)
MF C21 H14 O5



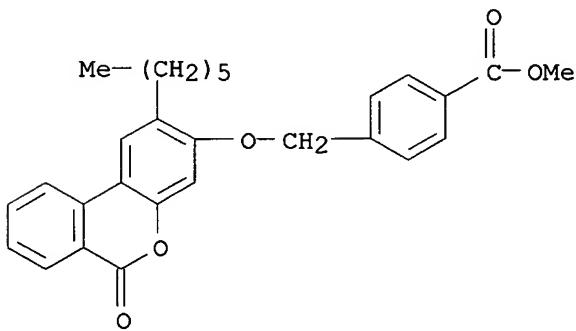
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl- (9CI)
MF C22 H16 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS
 IN Benzoic acid, 4-[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-,
 methyl ester (9CI)
 MF C28 H28 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus		SINCE FILE	TOTAL
COST IN U.S. DOLLARS		ENTRY	SESSION
FULL ESTIMATED COST		452.05	453.10

FILE 'CAPLUS' ENTERED AT 09:09:01 ON 27 JUN 2003
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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26
FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 16

REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 09:09:05 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.48 PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 58448 TO 65112
PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L6

L13 0 L12

=> 111
L14 0 L11

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 0.42 454.34

FILE 'CAPLUS' ENTERED AT 09:09:41 ON 27 JUN 2003
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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26

FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 111
L15 0 L11

=> file reg
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
0.42 454.76

FILE 'REGISTRY' ENTERED AT 09:10:33 ON 27 JUN 2003
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STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> search 19 sss full
FULL SEARCH INITIATED 09:10:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 65007 TO ITERATE

100.0% PROCESSED 65007 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.03

L16 6 SEA SSS FUL L9

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
148.15 602.91

FILE 'CAPLUS' ENTERED AT 09:11:00 ON 27 JUN 2003
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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26
FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 116
L17 0 L16

=> file reg
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
0.42 603.33

FILE 'REGISTRY' ENTERED AT 09:11:36 ON 27 JUN 2003
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STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e Benzoic acid, 4-(((6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy)methyl)-/cn
E1 1 BENZOIC ACID, 4-(((6-O-ACETYL-2,3,4-TRIS-O-(PHENYLMETHYL)-.A
LPHA.-D-MANNOPYRANOSYL)OXY)METHYL)-3-NITRO-, METHYL ESTER/CN
E2 1 BENZOIC ACID, 4-(((6-OXO-2,4-CYCLOHEXADIEN-1-YLIDENE)METHYL)
AMINO)-, METHYL ESTER/CN
E3 0 --> BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO,B,D)PYRAN-3-YL)OXY)METHY
L)-/CN
E4 1 BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D) PYRAN-3-YL)OXY)METHY
L)-/CN
E5 1 BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D) PYRAN-3-YL)OXY)METHY
L)-, METHYL ESTER/CN
E6 1 BENZOIC ACID, 4-(((6-QUINOXALINYLAMINO)THIOXOMETHYL)AMINO)-,
METHYL ESTER/CN
E7 1 BENZOIC ACID, 4-(((6R)-6-((2S)-2-(ACETYLAMINO)-1-OXO-3-(4-(
PHOSPHONOOXY)PHENYL)PROPYL)AMINO)TETRAHYDRO-5-OXO-1,4-THIAZE
PIN-4(5H)-YL)METHYL)-, 1-METHYL ESTER/CN
E8 1 BENZOIC ACID, 4-(((6R)-7-CARBOXY-6-HYDROXYHEPTYL)THIO)-/CN
E9 1 BENZOIC ACID, 4-(((6R)-TETRAHYDRO-5-OXO-6-((4-(PHOSPHONOOXY)
BENZOYL)AMINO)-1,4-THIAZEPIN-4(5H)-YL)METHYL)-, 1-METHYL EST
ER/CN
E10 1 BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7

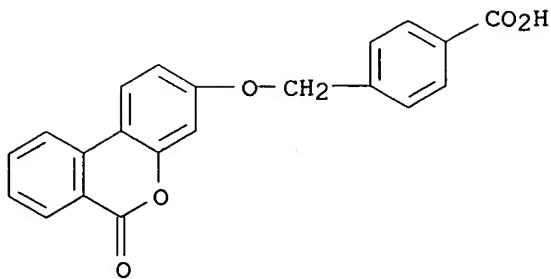
,12,12A-HEXAHYDRO-1,4-DIOXOPYRAZINO(1',2':1,6)PYRIDO(3,4-B)I
 NDOL-2(1H)-YL)METHYL)-/CN
 E11 1 BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7
 ,12,12A-HEXAHYDRO-1,4-DIOXOPYRAZINO(1',2':1,6)PYRIDO(3,4-B)I
 NDOL-2(1H)-YL)METHYL)-, METHYL ESTER/CN
 E12 1 BENZOIC ACID, 4-(((6S)-OCTAHYDRO-6-((4-HYDROXYPHENYL)METHYL)
 -2-METHYL-4,7-DIOXO-1-((PHENYLMETHYL)AMINO)CARBONYL)-8H-PYR
 AZINO(2,1-C)(1,2,4)TRIAZIN-8-YL)METHYL)-/CN

 => e Benzoic acid, 4-(((6-oxo-6H-dibenzo(b,d)pyran-3-yl)oxy)methyl)-/cn
 E1 1 BENZOIC ACID, 4-(((6-O-ACETYL-2,3,4-TRIS-O-(PHENYLMETHYL)-.ALPHA.-D-MANNOPYRANOSYL)OXY)METHYL)-3-NITRO-, METHYL ESTER/CN
 E2 1 BENZOIC ACID, 4-(((6-OXO-2,4-CYCLOHEXADIEN-1-YLIDENE)METHYL)
 AMINO)-, METHYL ESTER/CN
 E3 1 --> BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHYL)-/CN
 E4 1 BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHYL)-, METHYL ESTER/CN
 E5 1 BENZOIC ACID, 4-(((6-QUINOXALINYLAMINO)THIOXOMETHYL)AMINO)-,
 METHYL ESTER/CN
 E6 1 BENZOIC ACID, 4-(((6R)-6-((2S)-2-(ACETYLAMINO)-1-OXO-3-(4-(
 PHOSPHONOOXY)PHENYL)PROPYL)AMINO)TETRAHYDRO-5-OXO-1,4-THIAZE
 PIN-4(5H)-YL)METHYL)-, 1-METHYL ESTER/CN
 E7 1 BENZOIC ACID, 4-(((6R)-7-CARBOXY-6-HYDROXYHEPTYL)THIO)-/CN
 E8 1 BENZOIC ACID, 4-(((6R)-TETRAHYDRO-5-OXO-6-((4-(PHOSPHONOOXY)
 BENZOYL)AMINO)-1,4-THIAZEPIN-4(5H)-YL)METHYL)-, 1-METHYL EST
 ER/CN
 E9 1 BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7
 ,12,12A-HEXAHYDRO-1,4-DIOXOPYRAZINO(1',2':1,6)PYRIDO(3,4-B)I
 NDOL-2(1H)-YL)METHYL)-/CN
 E10 1 BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7
 ,12,12A-HEXAHYDRO-1,4-DIOXOPYRAZINO(1',2':1,6)PYRIDO(3,4-B)I
 NDOL-2(1H)-YL)METHYL)-, METHYL ESTER/CN
 E11 1 BENZOIC ACID, 4-(((6S)-OCTAHYDRO-6-((4-HYDROXYPHENYL)METHYL)
 -2-METHYL-4,7-DIOXO-1-((PHENYLMETHYL)AMINO)CARBONYL)-8H-PYR
 AZINO(2,1-C)(1,2,4)TRIAZIN-8-YL)METHYL)-/CN
 E12 1 BENZOIC ACID, 4-((6S,9.ALPHA.,11.ALPHA.,13E,15S)-6,9-EPOXY-
 11,15-DIHYDROXY-1-OXOPROSTA-7,13-DIEN-1-YL)AMINO)-/CN

 => e3
 L18 1 "BENZOIC ACID, 4-((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHYL)-
 "/CN

=> d 118

L18 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
 RN 314744-77-9 REGISTRY
 CN Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-
 (9CI) (CA INDEX NAME)
 MF C21 H14 O5
 SR Chemical Library
 LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> file chemcats		SINCE FILE	TOTAL
COST IN U.S. DOLLARS		ENTRY	SESSION
FULL ESTIMATED COST		7.10	610.43

FILE 'CHEMCATS' ENTERED AT 09:13:31 ON 27 JUN 2003
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FILE LAST UPDATED 21 JUNE 2003 (20030621UP)

For details on recent updates in CHEMCATS, enter NEWS FILE at an arrow prompt. For the list of suppliers currently in the file, enter HELP SPA, HELP SPBC, HELP SPDH, HELP SPIN, HELP SPOP, and HELP SPQZ. For the list of current catalogs, enter HELP CTA, HELP CTBC, HELP CTDH, HELP CTIN, HELP CTOP, and HELP CTQZ.

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CHEMCATS now contains more than 5 million records. See HELP CONTENT and NEWS FILE for details.

=> 116
 L19 22 L16

=> d 11911-22 ti
 'L1911-22' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'
 'TI' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'

The following are valid formats:

The default display format is IDE.

ALL ---- AN, CO, PD, ON, CN, RN, ST, Purity, Impurity, product identifiers, product notes, STR, product text (properties, regulatory information, references, prices, warnings, miscellaneous fields), CO, CA, CY, TX (products, terms, and conditions; products and services;

packaging and snipping; safety and handling; other supplier information)

COMP --- AN, CO, PD, CO, TX
IDE ---- AN, CO, PD, ON, CN, RN, LSF, ST, STR
MISC --- AN, miscellaneous product information fields
PINFO -- AN, pricing information text
PRICE -- AN, prices, quantities
PROD --- AN, product text
PROP --- AN, properties
REF ---- AN, references
REGS --- AN, regulatory information
SAFE --- AN, product warnings
SINFO -- AN, safety text
HIT ---- All fields containing hit terms
KWIC --- All hit terms plus 20 words on either side
OCC ---- List of display fields containing hit terms

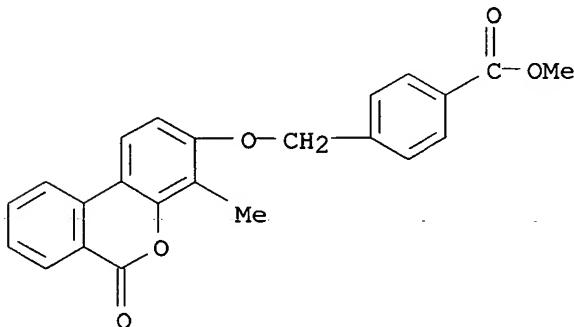
Hit terms will be highlighted in all displayable fields.

To display a particular field or fields, enter the display field codes. For a list of display field codes, enter 'HELP DFIELDS' at an arrow prompt (=>). Examples include: 'KWIC'; 'CN RN'; 'IDE CO'. You may specify the formats and fields in any order, and the information will be displayed in the same order as the format specification.

The same formats (except for HIT, KWIC, and OCC) may be used with the DISPLAY ACC command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (IDE):ide

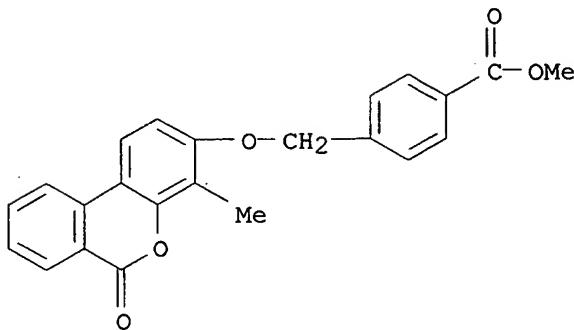
L19 ANSWER 1 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2003:2193953 CHEMCATS
Catalog Name (CO): ChemDiv, Inc. Product Library
Publication Date (PD): 25 Apr 2003
Order Number (ON): 3330-4466
Chemical Name (CN): Benzoic acid, 4-[[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester
CAS Registry No. (RN): 307551-62-8
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



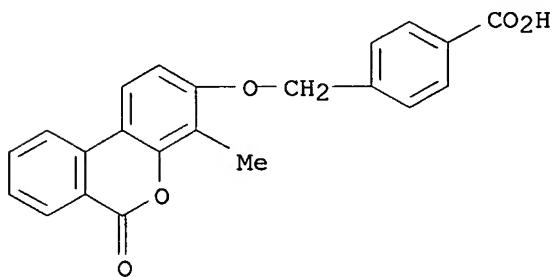
=> d 119 1-22 ide

L19 ANSWER 1 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2003:2193953 CHEMCATS
 Catalog Name (CO): ChemDiv, Inc. Product Library
 Publication Date (PD): 25 Apr 2003
 Order Number (ON): 3330-4466
 Chemical Name (CN): Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 CAS Registry No. (RN): 307551-62-8
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :

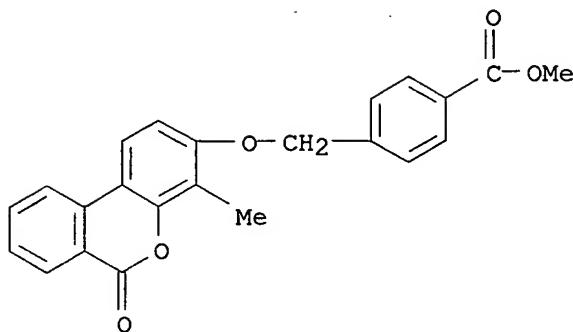


L19 ANSWER 2 OF 22 CHEMCATS COPYRIGHT 2003 ACS
 Accession No. (AN): 2003:884552 CHEMCATS
 Catalog Name (CO): Ambinter: Exploratory Library
 Publication Date (PD): 30 Apr 2003
 Order Number (ON): 7210430945
 Chemical Name (CN): Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-
 CAS Registry No. (RN): 314744-95-1
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :

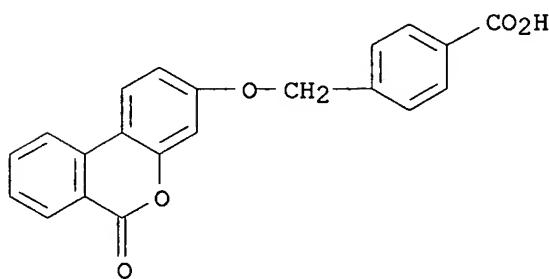


L19 ANSWER 3 OF 22 CHEMCATS COPYRIGHT 2003 ACS
 Accession No. (AN): 2003:884551 CHEMCATS
 Catalog Name (CO): Ambinter: Exploratory Library
 Publication Date (PD): 30 Apr 2003
 Order Number (ON): 7210430944
 Chemical Name (CN): Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 Synonym (CN): Also sold under Ambinter order number(s) F0398-0417, t0310-3431
 CAS Registry No. (RN): 307551-62-8

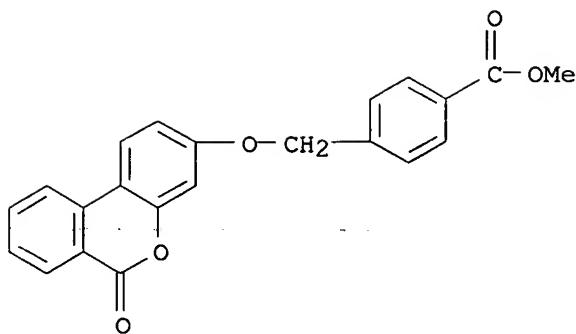
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L19 ANSWER 4 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2003:884511 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): 7210430903
Chemical Name (CN): Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-
CAS Registry No. (RN): 314744-77-9
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L19 ANSWER 5 OF 22 CHEMCATS COPYRIGHT 2003 ACS
Accession No. (AN): 2003:884510 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): 7210430902
Chemical Name (CN): Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
Synonym (CN): Also sold under Ambinter order number(s) F0398-0388
CAS Registry No. (RN): 307551-40-2
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



L19 ANSWER 6 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:2833186 CHEMCATS

Catalog Name (CO): Ambinter: Exploratory Library

Publication Date (PD): 30 Apr 2003

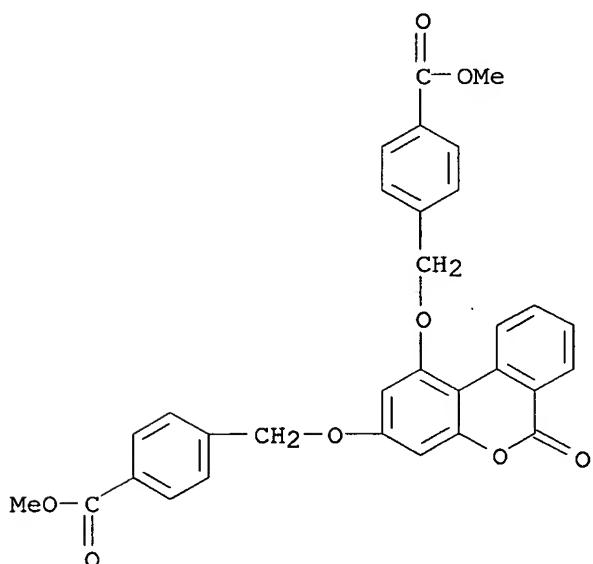
Order Number (ON): t0304-3777

Chemical Name (CN): Benzoic acid, 4,4'-(6-oxo-6H-dibenzo[b,d]pyran-1,3-diy)bis(oxymethylene)bis-, dimethyl ester

CAS Registry No. (RN): 438035-34-8

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :



L19 ANSWER 7 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:2800180 CHEMCATS

Catalog Name (CO): Interchim Intermediates

Publication Date (PD): 9 Jul 2002

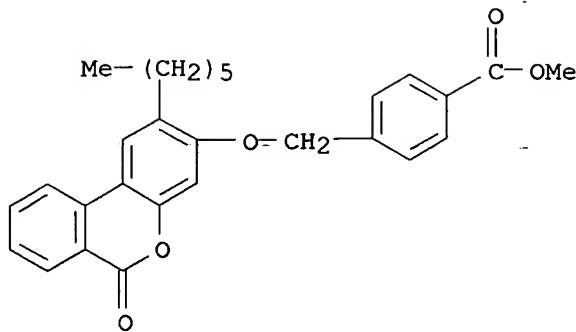
Order Number (ON): 7212010324

Chemical Name (CN): Benzoic acid, 4-[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester

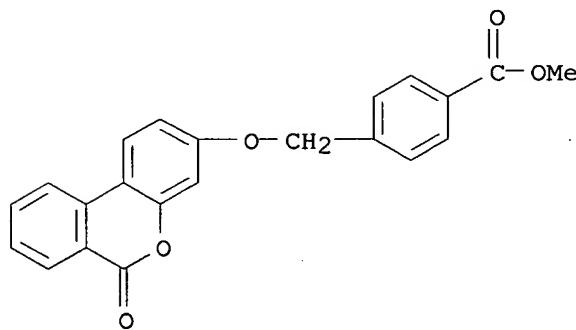
CAS Registry No. (RN): 405917-31-9

Supplementary Term (ST): CHEMICAL LIBRARY

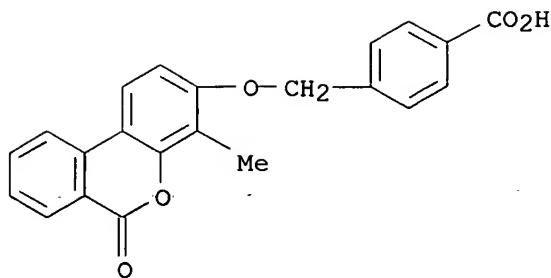
Structure :



L19 ANSWER 8 OF 22 CHEMCATS COPYRIGHT 2003 ACS
 Accession No. (AN): 2002:2796908 CHEMCATS
 Catalog Name (CO): Interchim Intermediates
 Publication Date (PD): 9 Jul 2002
 Order Number (ON): 7210430902
 Chemical Name (CN): Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 CAS Registry No. (RN): 307551-40-2
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :

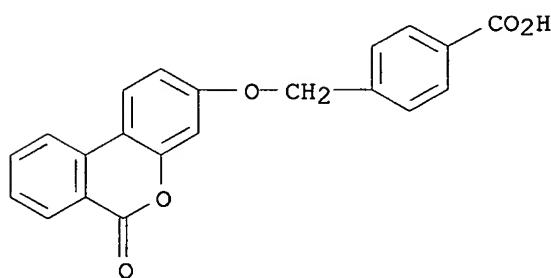


L19 ANSWER 9 OF 22 CHEMCATS COPYRIGHT 2003 ACS
 Accession No. (AN): 2002:2768171 CHEMCATS
 Catalog Name (CO): Interchim Intermediates
 Publication Date (PD): 9 Jul 2002
 Order Number (ON): 7210430945
 Chemical Name (CN): Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-
 CAS Registry No. (RN): 314744-95-1
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



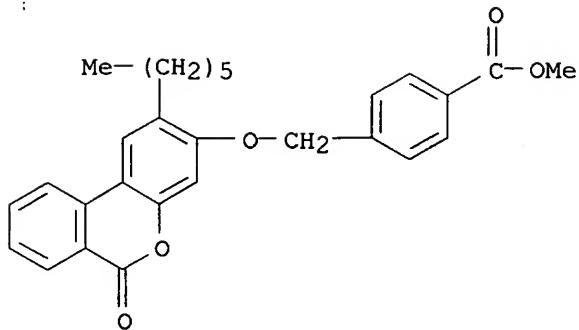
L19 ANSWER 10 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:2768153 CHEMCATS
Catalog Name (CO): Interchim Intermediates
Publication Date (PD): 9 Jul 2002
Order Number (ON): 7210430903
Chemical Name (CN): Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-
CAS Registry No. (RN): 314744-77-9
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



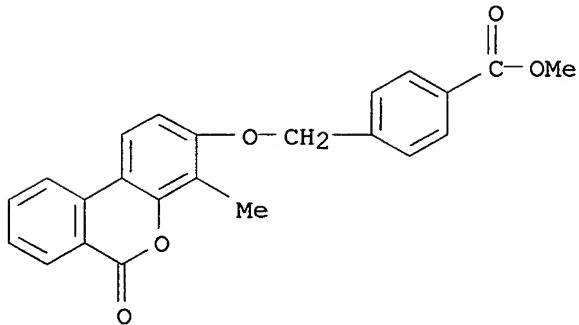
L19 ANSWER 11 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:2276618 CHEMCATS
Catalog Name (CO): Ambinter: Exploratory Library
Publication Date (PD): 30 Apr 2003
Order Number (ON): 7212010324
Chemical Name (CN): Benzoic acid, 4-[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
CAS Registry No. (RN): 405917-31-9
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :



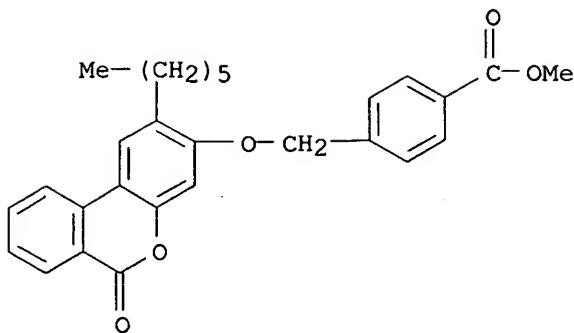
L19 ANSWER 12 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:2147072 CHEMCATS
 Catalog Name (CO): Interchim Intermediates
 Publication Date (PD): 9 Jul 2002
 Order Number (ON): 3330-4466
 Chemical Name (CN): Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 Synonym (CN): Also sold under Interchim order number(s) 7210430944, F0398-0417
 CAS Registry No. (RN): 307551-62-8
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



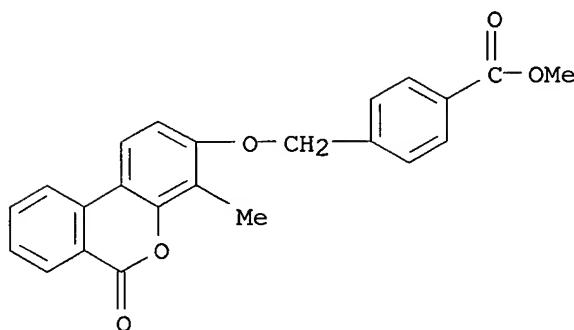
L19 ANSWER 13 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:1324350 CHEMCATS
 Catalog Name (CO): Otava Stock Chemicals
 Publication Date (PD): 28 May 2003
 Order Number (ON): 7212010324
 Chemical Name (CN): Benzoic acid, 4-[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 CAS Registry No. (RN): 405917-31-9
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



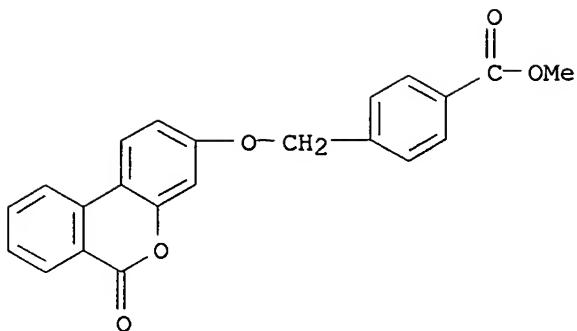
L19 ANSWER 14 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:607872 CHEMCATS
 Catalog Name (CO): ChemBridge Product List
 Publication Date (PD): 17 Jan 2002
 Order Number (ON): 6166000
 Chemical Name (CN): Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 CAS Registry No. (RN): 307551-62-8
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



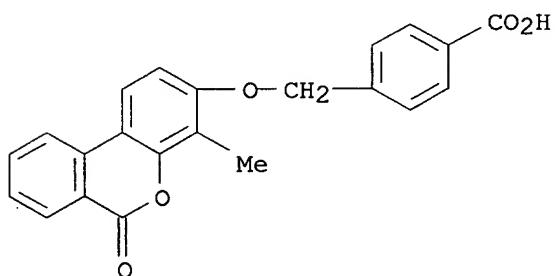
L19 ANSWER 15 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:605953 CHEMCATS
 Catalog Name (CO): ChemBridge Product List
 Publication Date (PD): 17 Jan 2002
 Order Number (ON): 6145952
 Chemical Name (CN): Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 CAS Registry No. (RN): 307551-40-2
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



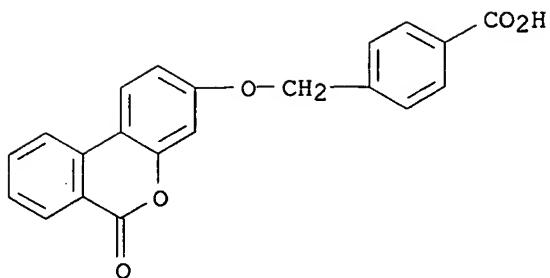
L19 ANSWER 16 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2001:131979 CHEMCATS
 Catalog Name (CO): Otava Chemical Collection
 Publication Date (PD): 21 Apr 2003
 Order Number (ON): 7210430945
 Chemical Name (CN): Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-
 CAS Registry No. (RN): 314744-95-1
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



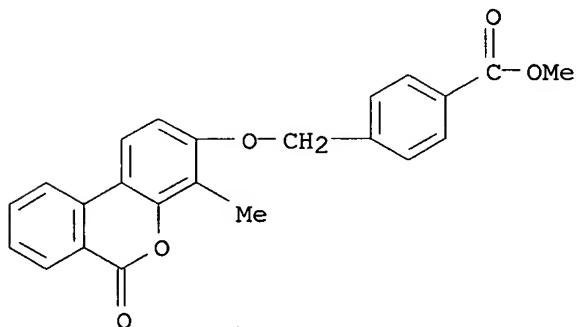
L19 ANSWER 17 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2001:131961 CHEMCATS
 Catalog Name (CO): Otava Chemical Collection
 Publication Date (PD): 21 Apr 2003
 Order Number (ON): 7210430903
 Chemical Name (CN): Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-
 CAS Registry No. (RN): 314744-77-9
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



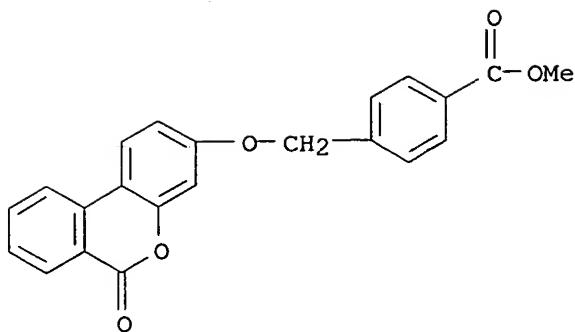
L19 ANSWER 18 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2000:1065757 CHEMCATS
 Catalog Name (CO): Otava Stock Chemicals
 Publication Date (PD): 28 May 2003
 Order Number (ON): 7210430944
 Chemical Name (CN): Benzoic acid, 4-[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 CAS Registry No. (RN): 307551-62-8
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



L19 ANSWER 19 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2000:1065735 CHEMCATS
 Catalog Name (CO): Otava Stock Chemicals
 Publication Date (PD): 28 May 2003
 Order Number (ON): 7210430902
 Chemical Name (CN): Benzoic acid, 4-[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl-, methyl ester
 CAS Registry No. (RN): 307551-40-2
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



L19 ANSWER 20 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2000:899357 CHEMCATS

Catalog Name (CO): SALOR

Publication Date (PD): 15 Jan 2003

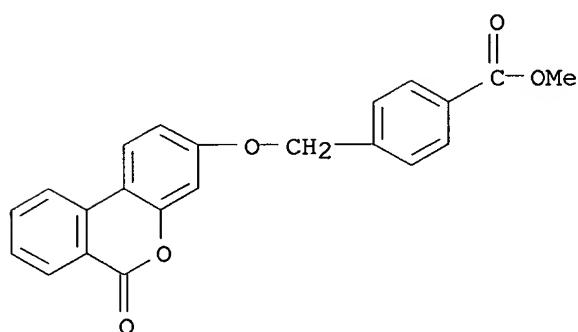
Order Number (ON): R632457

Chemical Name (CN): METHYL 4-(((6-OXO-6H-BENZO(C)CHROMEN-3-YL)OXY)METHYL)BENZOATE

CAS Registry No. (RN): 307551-40-2

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :



L19 ANSWER 21 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2000:897302 CHEMCATS

Catalog Name (CO): SALOR

Publication Date (PD): 15 Jan 2003

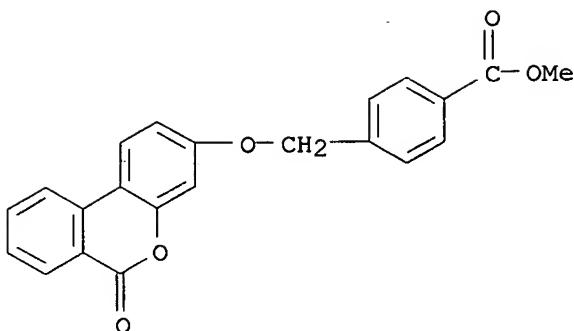
Order Number (ON): R609854

Chemical Name (CN): METHYL 4-(((6-OXO-6H-BENZO(C)CHROMEN-3-YL)OXY)METHYL)BENZOATE

CAS Registry No. (RN): 307551-40-2

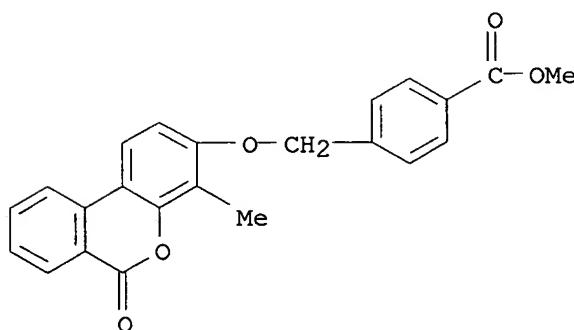
Supplementary Term (ST): CHEMICAL LIBRARY

Structure :



L19 ANSWER 22 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2000:434091 CHEMCATS
 Catalog Name (CO): SALOR
 Publication Date (PD): 15 Jan 2003
 Order Number (ON): R503738
 Chemical Name (CN): 4-(4-METHYL-6-OXO-6H-BENZO(C)CHROMEN-3-YLOXYMETHYL)-BENZOIC ACID METHYL ESTER
 CAS Registry No. (RN): 307551-62-8
 Supplementary Term (ST): CHEMICAL LIBRARY
 Structure :



=> logoff hold
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
43.20	653.63

SESSION WILL BE HELD FOR 60 MINUTES
 STN INTERNATIONAL SESSION SUSPENDED AT 09:16:46 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 Jun 03 New e-mail delivery for search results now available
NEWS 4 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 5 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN
NEWS 6 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 7 Sep 03 JAPIO has been reloaded and enhanced
NEWS 8 Sep 16 Experimental properties added to the REGISTRY file
NEWS 9 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 10 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11 Oct 24 BEILSTEIN adds new search fields
NEWS 12 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13 Nov 18 DKILIT has been renamed APOLLIT
NEWS 14 Nov 25 More calculated properties added to REGISTRY
NEWS 15 Dec 04 CSA files on STN
NEWS 16 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17 Dec 17 TOXCENTER enhanced with additional content
NEWS 18 Dec 17 Adis Clinical Trials Insight now available on STN
NEWS 19 Jan 29 Simultaneous left and right truncation added to COMPENDEX,
ENERGY, INSPEC
NEWS 20 Feb 13 CANCERLIT is no longer being updated
NEWS 21 Feb 24 METADEX enhancements
NEWS 22 Feb 24 PCTGEN now available on STN
NEWS 23 Feb 24 TEMA now available on STN
NEWS 24 Feb 26 NTIS now allows simultaneous left and right truncation
NEWS 25 Feb 26 PCTFULL now contains images
NEWS 26 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27 Mar 20 EVENTLINE will be removed from STN
NEWS 28 Mar 24 PATDPAFULL now available on STN
NEWS 29 Mar 24 Additional information for trade-named substances without
structures available in REGISTRY
NEWS 30 Apr 11 Display formats in DGENE enhanced
NEWS 31 Apr 14 MEDLINE Reload
NEWS 32 Apr 17 Polymer searching in REGISTRY enhanced
NEWS 33 Jun 13 Indexing from 1947 to 1956 added to records in CA/CAPLUS
NEWS 34 Apr 21 New current-awareness alert (SDI) frequency in
WPIDS/WPINDEX/WPIX
NEWS 35 Apr 28 RDISCLOSURE now available on STN
NEWS 36 May 05 Pharmacokinetic information and systematic chemical names
added to PHAR
NEWS 37 May 15 MEDLINE file segment of TOXCENTER reloaded
NEWS 38 May 15 Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39 May 16 CHEMREACT will be removed from STN
NEWS 40 May 19 Simultaneous left and right truncation added to WSCA
NEWS 41 May 19 RAPRA enhanced with new search field, simultaneous left and
right truncation
NEWS 42 Jun 06 Simultaneous left and right truncation added to CBNB
NEWS 43 Jun 06 PASCAL enhanced with additional data
NEWS 44 Jun 20 2003 edition of the FSTA Thesaurus is now available
NEWS 45 Jun 25 HSDB has been reloaded

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information

NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 13:10:23 ON 07 JUL 2003

=> file caplus
COST IN U.S. DOLLARS
SINCE FILE ENTRY TOTAL
SESSION
0.21 0.21
FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 13:10:30 ON 07 JUL 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 7 Jul 2003 VOL 139 ISS 2
FILE LAST UPDATED: 6 Jul 2003 (20030706/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> arotinoids
L1 54 AROTINOID

=> retinobenzoic
L2 40 RETINOBENZOIC

=> 11 and 12
L3 0 L1 AND L2

=> phenan?
T.4 62851 PHENAN?

=> 11 and 14

=> d 11 44-54 ti

1.1 ANSWER 44 OF 54 CAPTUS COPYRIGHT 2003 ACS

TI The effects of **arotinoids** on rat mammary carcinogenesis

L1 ANSWER 45 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Retinoid-induced changes of lipid synthesis in cultured human epidermal keratinocytes

L1 ANSWER 46 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Diazacholesterol-induced ichthyosis in the hairless mouse

L1 ANSWER 47 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Sulfur-containing **arotinoids**, a new class of retinoids

L1 ANSWER 48 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Synergistic effect of retinoic acid on DNA synthesis by prostaglandin F2.alpha. stimulated Swiss 3T3 cells

L1 ANSWER 49 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Effects of **arotinoids** upon murine embryonal carcinoma cells

L1 ANSWER 50 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Retinoic acid enhances the initiation of DNA synthesis stimulated by prostaglandin F2.alpha. in Swiss 3T3 cells

L1 ANSWER 51 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Affinity therapeutics. 1. Selective incorporation of 2-thiouracil derivatives in murine melanomas. Cytostatic activity of 2-thiouracil **arotinoids**, 2-thiouracil retinoids, **arotinoids**, and retinoids

L1 ANSWER 52 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology

L1 ANSWER 53 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Structure-activity relationship of retinoids in fetal rat bone cultures

L1 ANSWER 54 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI **Arotinoids**, a new class of highly active retinoids

=> d 11 52-54 ti fbib abs

L1 ANSWER 52 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology

AN 1982:141529 CAPLUS

DN 96:141529

TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology

AU Bollag, Werner

CS Pharma Res. Dep., F. Hoffmann-La Roche und Co. Ltd., Basel, Switz.

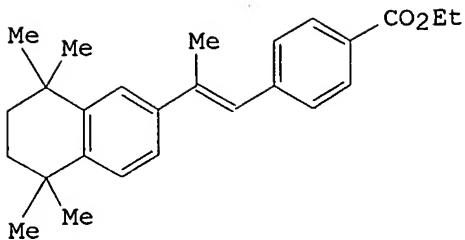
SO Cancer Chemotherapy and Pharmacology (1981), 7(1), 27-9

CODEN: CCPHDZ; ISSN: 0344-5704

DT Journal

LA English

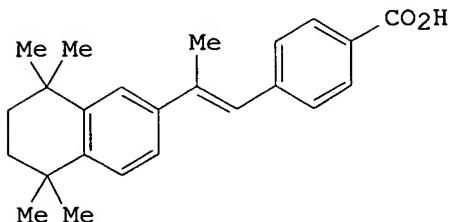
GI



I

AB **Arotinoids** are a new class of retinoids with particular biol. properties. Arotinoid Ro 13-6298 (I) [71441-09-3] in minute quantities leads to regression of chem. induced papillomas of the skin of mice. The ratio between the antipapilloma effect and the toxic syndrome of hypervitaminosis A is very favorable. Ro 13-6298 also has a therapeutic influence on chem. induced skin carcinomas in mice. As the papilloma model has proved to be suitable for screening for antipsoriatic and antikeratinizing properties as well as for antineoplastic screening, arotinoids might be useful in human clin. dermatol. and oncol.

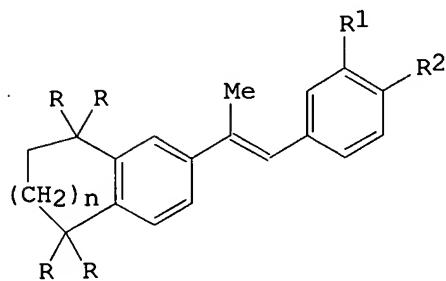
L1 ANSWER 53 OF 54 CAPLUS COPYRIGHT 2003 ACS
 TI Structure-activity relationship of retinoids in fetal rat bone cultures
 AN 1981:525879 CAPLUS
 DN 95:125879
 TI Structure-activity relationship of retinoids in fetal rat bone cultures
 AU Kistler, Andreas
 CS Biol. Pharm. Res. Dep., F. Hoffmann-La Roche Co. Ltd., Basel, CH-4002, Switz.
 SO Calcified Tissue International (1981), 33(3), 249-54
 CODEN: CTINDZ; ISSN: 0171-967X
 DT Journal
 LA English
 GI



I

AB The structure-activity relation of 29 retinoids was investigated in fetal rat bone organ cultures. Retinoids induced the release of proteoglycan followed by cartilage tissue breakdown. The loss of RNA was used as a parameter for cartilage resorption. During 6 days of incubation, RNA decreased up to 80% in the presence of active retinoids. The ED40 was detd. from dose-response curves of the various retinoids. The new compds., called **arotinoids**, which contained the retinoic acid C skeleton in a fixed cisoid geometric conformation, were up to 200 times more active than all-trans-beta-retinoic acid. The most active compd. was I [71441-28-6]. Several lines of evidence indicated that the carboxylic acid end group was essential for the activity of retinoids in fetal bone cultures. These new, highly active retinoids might be an excellent tool to investigate whether the retinoid action is mediated by specific cellular retinoid binding proteins.

L1 ANSWER 54 OF 54 CAPLUS COPYRIGHT 2003 ACS
 TI **Arotinoids**, a new class of highly active retinoids
 AN 1980:586020 CAPLUS
 DN 93:186020
 TI **Arotinoids**, a new class of highly active retinoids
 AU Loeliger, Peter; Bollag, Werner; Mayer, Hans
 CS F. Hoffmann-La Roche and Co. Ltd., Basel, CH 4002, Switz.
 SO European Journal of Medicinal Chemistry (1980), 15(1), 9-15
 CODEN: EJMCA5; ISSN: 0009-4374
 DT Journal
 LA English
 GI



AB A new class of retinoids, named **arotinoids** (I), R = H or Me, R1 = H, R2 = COEt, n = 0; R = R1 = Me, R2 = CO2Et, n = 1; R = Me, R1 = H, R2 = H, Me, CHO, CH2OH, CH2OMe, CH2OAc, CO2H, CO2Et, CO2CHMe2, CO2CMe3 or CONHET, n = 1), which had up to 10 times more favorable therapeutic ratio for papilloma regression than retinoic acid (II) were prep'd. by the Wittig reaction of (1-arylethyl)triphenylphosphonium bromides with benzaldehydes. E.g., Me 5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthyl ketone was reduced, the alc. converted to the bromide, and this was quaternized with Ph3P and reacted with 4-HCOC6H4CO2Et to give (E)-I (R = Me, R1 = H, R2 = CO2Et, n = 1), which had therapeutic potency in the antipapilloma test 8000 times that of II while the toxic hypervitaminosis A effects were increased by 800 times.

=> tricyc?
 L6 30539 TRICYC?

=> d his

(FILE 'HOME' ENTERED AT 13:10:23 ON 07 JUL 2003)

FILE 'CAPLUS' ENTERED AT 13:10:30 ON 07 JUL 2003

L1 54 AROTINOIDS
 L2 40 RETINOBENZOIC
 L3 0 L1 AND L2
 L4 62851 PHENAN?
 L5 0. L1 AND L4
 L6 30539 TRICYC?

=> l1 and l6
 L7 0 L1 AND L6

=> ?arotinoids
 L8 298 ?AROTINOIDS

=> carotinoids

=> 18 not 19

L10 89 L8 NOT L9

=> 110 not 11

L11 35 L10 NOT L1

=> benzo?

L12 475881 BENZO?

=> 111 and 112

L13 15 L11 AND L12

=> d 113 1-15 ti

L13 ANSWER 1 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties

L13 ANSWER 2 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions

L13 ANSWER 3 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-**benzo[b]thien-5-yl**)-1-propenyl]**benzoate**, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-**benzofuranyl**)-1-propenyl]**benzoate**, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-3-hydroxy-1-propenyl]**benzoate** as potential metabolites of selected **heteroarotinoids** with fused five-membered rings

L13 ANSWER 4 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic cultures of ovarian carcinoma

L13 ANSWER 5 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI Synthesis, Structure-Activity Relationships, and RAR. γ -Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]

L13 ANSWER 6 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran-6-yl**)-1-propenyl]**benzoic acid-11-[14C]**

L13 ANSWER 7 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI Synthesis, Structure-Activity Relationships, and RAR. γ -Ligand Interactions of Nitrogen **Heteroarotinoids**

L13 ANSWER 8 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI synthesis, receptor specificity and TGase activity of **heteroarotinoids**-anticancer-agents

L13 ANSWER 9 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

L13 ANSWER 10 OF 15 CAPIUS COPYRIGHT 2003 ACS

TI **Heteroarotinoids**: crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl]**benzoate**

L13 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Novel **heteroarotinoids**: synthesis and biological activity

L13 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids**: analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples

L13 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Heteroarotinoid compounds as anticancer agents

L13 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids**. Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells

L13 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]**benzoate**

=> benzoarotinoid?

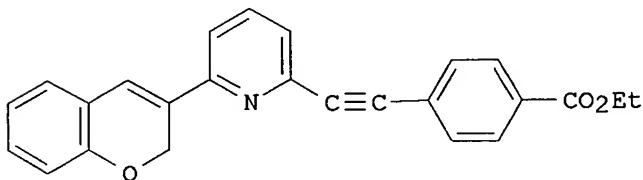
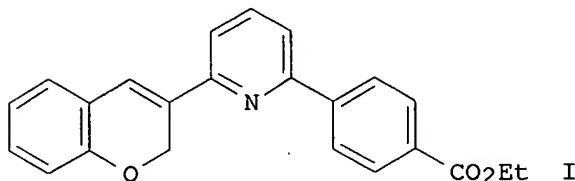
L14 0 BENZOAROTINOID?

=> d 113 1-15 ti fbib abs

L13 ANSWER 1 OF 15 CAPIUS COPYRIGHT 2003 ACS
TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties
AN 2003:322782 CAPLUS
TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties
AU Weerasekare, G. Mahika; Berlin, K. Darrell; Sunkara, Haribabu; Ford, Warren T.
CS Oklahoma State University, Stillwater, OK, USA
SO Phosphorus, Sulfur and Silicon and the Related Elements (2003), 178(5), 993-1006
CODEN: PSSLEC; ISSN: 1042-6507
PB Taylor & Francis Ltd.
DT Journal
LA English
AB Synthetic methods were developed to prep. Et (E)-4-[2-(3,4-dihydro-2-n-octyl-1-oxy-2H-1-**benzothio**-pyran-6-yl)-1-propenyl]**benzoate** (1) and Et (E)-4-[2-(3,4-dihydro-2-n-octyl-2H-1-**benzothiopyran**-6-yl)-1-propenyl]**benzoate** (10). These are the first examples of **heteroarotinoids** which possess properties of liq. crystals. The properties were evaluated using differential scanning calorimetry and by use of polarizing microg. Both displayed textures which are typical of a smectic or cholesteric phase.

L13 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions
AN 2001:867362 CAPLUS
DN 136:151322
TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions
AU Alami, Mouad; Peyrat, Jean-Francois; Belachmi, Larbi; Brion, Jean-Daniel
CS Laboratoire de Chimie Therapeutique, associe au CNRS (BioCIS), Universite

SO Paris-Sud, Faculte de Pharmacie, Chatenay-Malabry, 92296, Fr.
European Journal of Organic Chemistry (2001), (22), 4207-4212
CODEN: EJOCFK; ISSN: 1434-193X
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
OS CASREACT 136:151322
GI



II

AB A convergent synthesis of **heteroarotinoids** bearing chromene rings in assocn. with pyridyl or ethynylpyridyl moieties, from 6-bromo-2-pyridylzinc chloride is described. This new functional heteroarylzinc reagent, readily accessible from 2,6-dibromopyridine, may undergo a selective palladium-catalyzed carbon-carbon bond-forming reaction to yield the corresponding 6-substituted-2-bromopyridines. Further manipulation of the remaining bromine atom to give the zinc deriv., and subsequent coupling with Et 4-iodobenzoate under palladium catalysis conditions afforded heteroarotinoid I. Coupling of the 6-substituted-2-bromopyridines or Me nicotinate triflate with appropriate alkynes under Sonogashira conditions give the corresponding **heteroarotinoids**, e.g. II.

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-benzo[b]thien-5-yl)-1-propenyl]benzoate, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-benzofuranyl)-1-propenyl] benzoate, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-benzofuranyl)-3-hydroxy-1-propenyl]benzoate as potential metabolites of selected **heteroarotinoids** with fused five-membered rings

AN 2001-691383 -CAPLUS

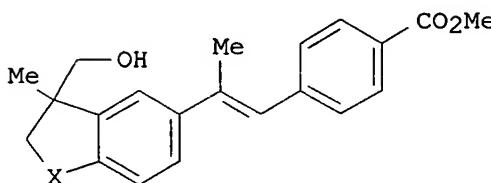
DN 136:5846

TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-benzo[b]thien-5-yl)-1-propenyl]benzoate, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-benzofuranyl)-1-propenyl] benzoate, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-benzofuranyl)-3-hydroxy-1-propenyl]benzoate as potential metabolites of selected **heteroarotinoids** with fused five-membered rings

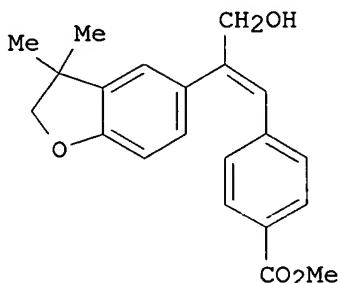
AU Gale, Jonathan B.; Klucik, Jozef; Subramanian, Shankar; Berlin, K. Darrell
CS Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078,

USA

SO Organic Preparations and Procedures International (2001), 33(5), 487-499
CODEN: OPPIAK; ISSN: 0030-4948
PB Organic Preparations and Procedures, Inc.
DT Journal
LA English
OS CASREACT 136:5846
GI



I



II

AB The title compds. I (X = S), I (X= O), and II were prep'd. were prep'd. starting from 2-aminothiophenol and 2-nitrophenol.

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

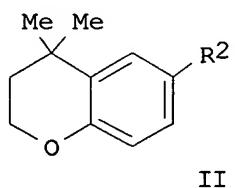
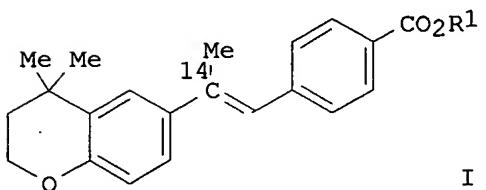
L13 ANSWER 4 OF 15 CAPIUS COPYRIGHT 2003 ACS
TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic cultures of ovarian carcinoma
AN 2001:308164 CAPIUS
DN 135:251521
TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic cultures of ovarian carcinoma
AU Guruswamy, Suresh; Lightfoot, Stan; Gold, Michael A.; Hassan, Raffit; Berlin, K. Darrell; Ivey, R. Todd; Benbrook, Doris M.
CS Departments of Obstetrics and Gynecology and Biochemistry and Molecular Biology, University of Oklahoma Health Sciences Center, Oklahoma City, OK, 73190, USA
SO Journal of the National Cancer Institute (2001), 93(7), 516-525
CODEN: JNCIEQ; ISSN: 0027-8874
PB Oxford University Press
DT Journal
LA English
AB Background: Retinoic acid analogs, called retinoids, have shown promise in clin. trials in preventing breast and ovarian cancers. Classic retinoids bind to retinoic acid receptors, which regulate cell growth. Some novel retinoids, such as fenretinide, i.e., N-(4-hydroxyphenyl)retinamide (4-HPR), induce apoptosis through retinoic acid receptor-independent mechanisms; however, they appear to do so only at concns. above those achieved in clin. chemoprevention trials. At lower concns. ($\text{.1 to } \text{req. 1 } \mu\text{M}$), 4-HPR acts like classic retinoids, by inducing differentiation

through a receptor-dependent mechanism. Our goal was to compare the effects of novel receptor-independent (apoptotic) retinoids with those of classic growth-inhibitory retinoids at clin. achievable doses on growth, differentiation, and apoptosis in ovarian tissue. Methods: Four receptor-independent (apoptotic) and seven growth-inhibitory retinoids, including synthetic, low-toxicity compds. called **heteroarotinoids**, were administered at concns. of 1 .mu.M to organotypic cultures of ovarian primary and cancer cell lines: OVCAR-3, Caov-3, and SK-OV-3. After fixation, embedding, and sectioning, the growth fraction was quantified by measuring expression of the proliferation marker Ki-67/myb, differentiation was assessed by expression of mucin, and apoptosis was evaluated by the TUNEL assay. Spearman correlation anal. was performed on the data, and all P values were two-sided. Results: All 11 retinoids reversed characteristics assocd. with the cancerous phenotype in all neoplastic cultures. Glandular structures were obsd. consistently in retinoid-treated, but not in untreated, OVCAR-3 and Caov-3 cultures. All retinoids decreased growth fractions, and some increased mucin expression. All receptor-independent retinoids and two receptor-dependent retinoids induced apoptosis, and the induction correlated significantly with increased expression of the mucin MUC1 ($r = .83$; $P = .03$). Retinoids with ester-linking groups did not induce apoptosis but decreased the growth fraction in correlation with MUC1 induction ($r = -.93$; $P = .02$). Conclusions: At clin. achievable concns., all retinoids tested decrease the growth fraction, induce differentiation and apoptosis. Induction of MUC1 expression is implicated in the mechanisms of action.

RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS
 TI Synthesis, Structure-Activity Relationships, and RAR. γ -Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]
 AN 1999:803609 CAPLUS
 DN 132:293893
 TI Synthesis, Structure-Activity Relationships, and RAR. γ -Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]
 AU Dhar, Arindam; Liu, Shengquan; Klucik, Jozef; Berlin, K. Darrell; Madler, Matora M.; Lu, Shennan; Ivey, R. Todd; Zacheis, David; Brown, Chad W.; Nelson, E. C.; Birckbichler, Paul J.; Benbrook, Doris M.
 CS Departments Obstetrics Gynecology of Biochem., Molecular Biol. of Otorhinolaryngology and Urology, Univ. Oklahoma Health Sciences Center, Oklahoma City, OK, 73190, USA
 SO Journal of Medicinal Chemistry (2000), 43(2), 303
 CODEN: JMCMAR; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 AB On page 3606, under Discussion, lines 24 and 25, the ref. to Table 2 is incorrect; Table 1 is the correct ref. The cor. sentence is as follows: "The EC50 value of 6 nM and the 103% efficacy of 2 (Table 1), in comparison to that of 9-c-RA, indicate that 2 may be useful as a pharmaceutical agent for disorders of the skin."
 L13 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS
 TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic acid**-11-[14C]
 AN 1999:525825 CAPLUS
 DN 131:310738
 TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic acid**-11-[14C]
 AU Liu, Shengquan; Berlin, K. Darrell; Simms-Kelley, Melissa D.; Nelson, Eldon C.; Benbrook, Doris M.

CS Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078,
 USA
 SO Journal of Labelled Compounds & Radiopharmaceuticals (1999), 42(8),
 789-796
 CODEN: JLCRD4; ISSN: 0362-4803
 PB John Wiley & Sons Ltd.
 DT Journal
 LA English
 GI

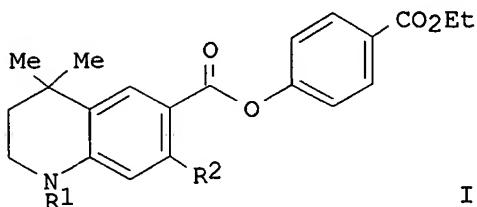


AB **Heteroarotinoids** may be useful in the treatment of skin disorders and a wide variety of cancers. A synthesis of the C-14 labeled heteroarotinoid, (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzopyran-6-yl)-1-propenyl]benzoic acid-11-[14C] (I; R1 = H) is described via a multistep procedure similar to that used to obtain the unlabeled compd. The latter has shown good activity in several assays compared to the std. trans-retinoic acid. Redn. of the carbonyl group in 4,4-dimethylchroman-6-yl Me ketone-(carbonyl-14C) (II; R2 = 13COMe) with LiAlH4 gave alc. II (R2 = 13CHMeOH). Phosphorylation with triphenyl-phospine hydrobromide in methanol led to the corresponding phosphonium salt II (R2 = 13CHMeP+Ph3Br-). Addn. of n-butyllithium to II (R2 = 13CHMeP+Ph3Br-) in ether at -78.degree.C generated the Wittig reagent in situ and to this was added Et 4-formylbenzoate. Workup and chromatog. afforded E-ester I (R1 = Me) and the Z-ester which were both hydrolyzed to labeled I. Labeled I was identical to the unlabeled isotopomer in terms of spectral data and m.p. The specific activity of I was detd. to be 57.2 .mu.Ci/mg.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS
 TI -Synthesis, -Structure-Activity Relationships,- and -RAR. gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**
 AN 1999:521109 CAPLUS
 DN 131:310737
 TI Synthesis, Structure-Activity Relationships, and RAR. gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**
 AU Dhar, Arindam; Liu, Shengquan; Klucik, Jozef; Berlin, K. Darrell; Madler, Matora M.; Lu, Shennan; Ivey, R. Todd; Zacheis, David; Brown, Chad W.; Nelson, E. C.; Birckbichler, Paul J.; Benbrook, Doris M.
 CS Departments of Obstetrics Gynecology of Biochemistry Molecular Biology of Otorhinolaryngology and of Urology, University of Oklahoma Health Sciences

SO Center, Oklahoma City, OK, 73190, USA
Journal of Medicinal Chemistry (1999), 42(18), 3602-3614
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



AB Three **heteroarotinoids** contg. a nitrogen atom in the first ring and a C-O linking group between the two aryl rings were synthesized and evaluated for RAR and RXR retinoid receptor transactivation, tumor cell growth inhibition, and transglutaminase (TGase) induction. Et 4-(N,4,4-trimethyl-1,2,3,4-tetrahydroquinolinyl)benzoate (I; R1 = Me, R2 = H) contained an N-CH3 group and activated all retinoid receptors except for RAR. γ . Increasing the hydrophobicity around the rings with analogs Et 4-(N,4,4,7-tetramethyl-1,2,3,4-tetrahydroquinolin-6-oyloxy)benzoate (I; R1 = R2 = Me) and Et 4-(4,4-dimethyl-N-isopropyl-1,2,3,4-tetrahydroquinolin-6-oyloxy)benzoate (I; R1 = CHMe2, R2 = H) increased the potency and specificity for RAR. α ., RAR. β ., and RXR. α ., compared to I (R1 = Me, R2 = H), but had little effect on RXR. β . and RXR. γ . activation. Although I (R1 = Me, CHMe2, R2 = H) were unable to activate RAR. γ ., I (R1 = R2 = Me) did activate this receptor with efficacy and high potency equal to that of 9-cis-retinoic acid (II). All three **heteroarotinoids** exhibited 5-8-fold greater specificities for RAR. β . over RAR. α .. In addn., esters I inhibited the growth of two cell lines each derived from cervix, vulvar, ovarian, and head/neck tumors with similar efficiencies to that of II through a mechanism independent of apoptosis. The vulvar cell lines were the most sensitive, and the ovarian lines were the least sensitive. Ester was similar to I (R1 = Me, CHMe2; R2 = H) except that I (R1 = R2 = Me) was a much more potent growth inhibitor of the two vulvar cell lines, which is consistent with strong RAR. γ . activation by I (R1 = R2 = Me) [but not by I (R1 = Me, CHMe2; R2 = H)] and the high levels of RAR. γ . expression in skin. All three **heteroarotinoids** induced prodn. of TGase, a marker of retinoid activity in human erythroleukemic cells. Esters I (R1 = R2 = Me; R1 = CHMe2, R2 = H) were the more potent TGase activators than I (R1 = Me R2 = H), in agreement with the stronger activation of the RAR receptors by I (R1 = R2 = Me; R1 = CHMe2, R2 = H). The biol. activities of these agents, and the RAR. γ . potency of I (R1 = R2 = Me) in particular, demonstrate the promise of these compds. as pharmaceutics for cancer and skin disorders.

- RE.CNT 40-- THERE ARE 40 CITED-REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI synthesis, receptor specificity and TGase activity of
heteroarotinoids-anticancer agents
AN 1998:147324 CAPLUS
DN 128:204998
TI synthesis, receptor specificity and TGase activity of
heteroarotinoids-anticancer agents
IN Berlin, Kenneth Darrel; Subramanian, Shanker; Nelson, Eldon Carl; Madler,

Matora May; Patterson, Manford Kenneth, Jr.; Birckbichler, Paul Joseph;
Benbrook, Doris Mangiaracina

PA Board of Regents for Oklahoma State University, USA

SO PCT Int. Appl., 93 pp.

CODEN: PIXXD2

DT Patent

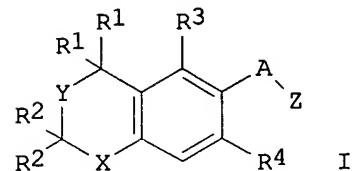
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9807716	A2	19980226	WO 1997-US14720	19970821
	W: AU, CA, CN, JP			US 1996-24521P P	19960823
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9740805	A1	19980306	AU 1997-40805	19970821
				US 1996-24521P P	19960823
				WO 1997-US14720W	19970821

OS MARPAT 128:204998

GI



AB Synthesis of heteroarotinoid structures (I) [R1 = H, Me; R2 = H, Me; R3 = H, Me; R4 = H, Me, OMe; A = CO2, O2C, CONOH, CONOMe, NHCO, C(Me)=CH, COCH=CH; X = O, S, SO, SO2, NMe, NET, NPr, NCHMe2, CMe2; Y = CH2, O, S; Z = C6H4-4-CO2R, C6H4-3-CO2R, C6H3-3-Me-4-CO2R, C6H3-2-Me-4-CO2R, CH=CHCH=CHCO2R, CH=CHC(Me)=CHCO2R; R = H, Me, Et, Pr, CHMe2] partially related to trans-retinoic acid through the basic, fused-ring framework and having receptor specificity as well as activity in stimulating formation of the enzyme transglutaminase as a marker for anticancer activity is reported. Thus, I (R1=R2 = Me, R3=R4 = H, Y = CH2, X = S, A = NHCO, Z = C6H3-2-Me-4-CO2R, R = H) (II) is prep'd. in 68% yield by NaOH hydrolysis of the corresponding ester in ethanol formed by the condensation of 6-amino-2,3-dihydro-2,2,4,4-tetramethyl-2H-1-benzothiopyran with monomethyl terephthaloyl chloride. II shows an R value of 0.76 as compared to trans-retinoic acid in TGase assay.

L13 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

AN 1997:638457 CAPLUS

DN 127:307506

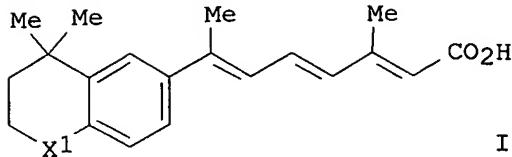
TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

AU Benbrook, Doris M.; Madler, Matora M.; Spruce, Lyle W.; Birckbichler, Paul J.; Nelson, Eldon C.; Subramanian, Shankar; Weerasekare, G. Mahika; Gale, Jonathan B.; Patterson, Manford K., Jr.; Wang, Binghe; Wang, Wei; Lu, Shennan; Rowland, Tami C.; DiSivestro, Paul; Lindamood, Charles; Hill, Donald L.; Berlin, K. Darrell

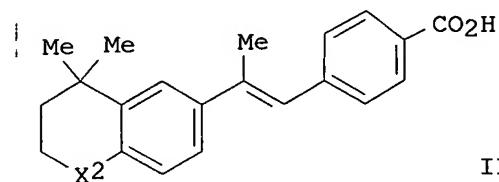
CS Departments of Obstetrics Gynecology Urology and Medicinal Chemistry and Pharmaceutics, University of Oklahoma Health Sciences Center, Oklahoma City, OK, 73190, USA

SO Journal of Medicinal Chemistry (1997), 40(22), 3567-3583

PB CODEN: JMCMAR; ISSN: 0022-2623
DT American Chemical Society
LA Journal
GI English



I

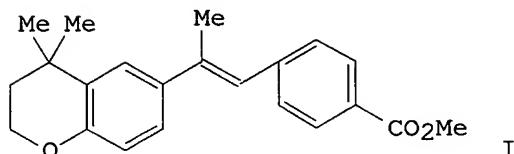


II

AB A series of retinoids, contg. heteroatoms in a cyclic ring and called **heteroarotinoids**, were synthesized, and their biol. activity was evaluated using tissue culture lines that have measurable responses to trans-retinoic acid (t-RA). Transglutaminase (TGase) was assessed in the human erythroleukemia cell line (GM06141A) as an indicator of differentiation and apoptosis. Proliferation was evaluated in a human cervical cell line, CC-1, which exhibits dose-dependent alterations in growth rate in response to treatment with trans-retinoic acid. Activation of nuclear retinoic acid receptors was detd. in a reporter cell line established from CC-1. The reporter line, called CC-B, contains a reporter gene controlled by a retinoic acid responsive element (RARE) and a thymidine kinase (tk) promoter. Treatment of the CC-B line with the **heteroarotinoids** resulted in a dose-responsive and retinoid-dependent regulation of reporter gene expression. The **heteroarotinoids** exhibited activity in all assays and correlated in a statistically significant manner between assays. RARE transactivation activity in CC-B cells correlated with induction of TGase in GM06141A ($R = 0.96$) and with a decrease in the growth rate of CC-1 cells ($R = -0.90$). The ability of the selected **heteroarotinoids** to induce differentiation, inhibit proliferation, and activate nuclear receptors demonstrates the chemotherapeutic potential of these agents. In view of the biol. activity cited, an in vivo toxicity study was conducted on male B6D2F1 mice with three **heteroarotinoids**, namely (2E,4E,6E)-3,7-dimethyl-7-(1,2,3,4-tetrahydro-4,4-dimethylthiochroman-6-yl)-2,4,6-heptatrienoic acid (I; $X1 = S$), (2E,4E,6E)-3,7-dimethyl-7-(1,2,3,4-tetrahydro-4,4-dimethylchroman-6-yl)-2,4,6-heptatrienoic acid (I; $X1 = O$), and (E)-p-[2-(4,4-dimethylchroman-6-yl)propenyl]benzoic acid (II; $X2 = O$). The mice were used with gavage of **heteroarotinoids** in corn oil [0.1, 0.2, 0.4, or 0.8 mg/kg] and with 0.01 or 0.05 mg/kg of (E)-4-[2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-1-propenyl]benzoic acid [TTNPB (II; $X2 = CMe_2$)] as ref. controls. The target organs affected in the mice by the three **heteroarotinoids** were those typically assocd. with trans-retinoic acid (III) toxicity. The max. tolerated dose (MTD) of III was 9.4 mg/kg/day, which was equal in toxicity to that of III and 1000-fold less toxic than TTNPB. The MTDs of I were 34 and 32 mg/kg/day,

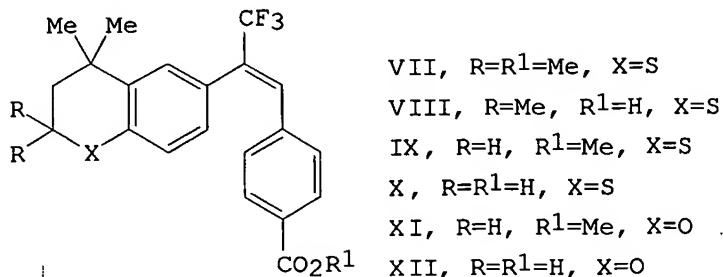
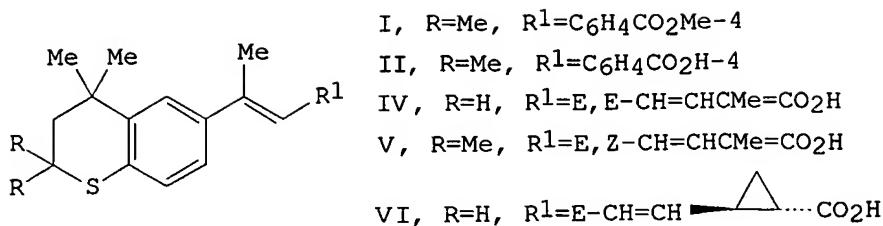
resp., which is 3-fold less toxic than III and 3000-fold less toxic than TTNPB. The 3000-fold reduced toxicity, compared with only a 27% redn. biol. activity of I with respect to that of TTNPB, obsd. in our assays indicates a good therapeutic ratio of these **heteroarotinoids** over the parent compd. The biol. activity and reduced toxicity of these **heteroarotinoids** demonstrate the potential efficacy as anticancer agents.

L13 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS
 TI **Heteroarotinoids:** crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl] benzoate
 AN 1992:6745 CAPLUS
 DN 116:6745
 TI **Heteroarotinoids:** crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl] benzoate
 AU Welsh, William J.; Cody, Vivian; Suwinski, Kinga; Berlin, K. Darrell; Rajadhyaksha, Shirish N.; Subramanian, Shankar; Verma, A. K.
 CS Dep. Chem., Univ. Missouri, St. Louis, MO, 63121, USA
 SO Structural Chemistry (1991), 2(5), 515-22
 CODEN: STCHES; ISSN: 1040-0400
 DT Journal
 LA English
 GI



AB Crystal structures and MM2P mol. mechanics force-field and AM1 MO calcns. were performed on Me (E)- and Me (Z)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl]benzoate (I) and confirmed that the calcd. mol. structures are in good agreement with the obsd. crystallog. conformations which show that both isomers have a twist-sofa oxo ring conformation and nearly perpendicular arom. ring systems, resp. Full relaxation MM2P conformational energy profiles for the rotation about the propenyl bridge indicate that the max. energy barrier is less than 3.5 kcal/mol.

L13 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS
 TI Novel **heteroarotinoids:** synthesis and biological activity
 AN 1991:114595 CAPLUS
 DN 114:114595
 TI Novel **heteroarotinoids:** synthesis and biological activity
 AU Spruce, Lyle W.; Gale, Jonathan B.; Berlin, K. Darrell; Verma, A. K.; Breitman, Theodore R.; Ji, Xinhua; Van der Helm, Dick
 CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA
 SO Journal of Medicinal Chemistry (1991), 34(1), 430-9
 CODEN: JMCMAR; ISSN: 0022-2623
 DT Journal
 LA English
 OS CASREACT 114:114595
 GI



AB Thirteen **heteroarotinoids** were synthesized. The key step in each prepn. was the condensation of the appropriate chroman-, thiochroman-, or **benzothienyl**-substituted phosphorus ylide, obtained from the independent synthesis of the corresponding phosphonium salts, with selected polyene-substituted aldehyde esters. Screening of the compds. was with one of two assays. One assay measured the ability of a retinoid to inhibit the phorbol ester induced increase of mouse epidermal ornithine decarboxylase (ODC) activity. The other assay measured retinoid-induced differentiation of the human myeloid leukemia cell line HL-60. In the ODC assay, all thirteen compds. were screened. The most active **heteroarotinoids** were ester I and the acid II. Both of these retinoids had ID₅₀ values (dose required for half-maximal inhibition of phorbol ester induced ODC activity) of about 0.3 nmol. In comparison, the ID₅₀ value for trans-retinoic acid III was 0.12 nmol while the ID₅₀ values for acids IV and V were about 3.5 nmol. **Heteroarotinoids** VI and VII-XII had ID₅₀ values of 35 nmol or greater. With a thiochroman unit, the most active acids in decreasing order of activity in the ODC assay were II > V > VI. Thus, simple replacement of the terminal propenyl system [C(16,17,18)] in IV with a cyclopropyl group produced acid VI with markedly reduced activity. With a **benzoic** acid group as part of the structure attached to the thiochroman unit, the ODC activity was enhanced as shown in I and II. The combination of the 2,2,4,4-tetramethylthiochroman group and the **benzoic** acid (or ester) terminal group seemed to enhance the biol. action which resembles that found with (E)-4-[2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-1-propenyl]**benzoic** acid, a well-known model system. Replacing the protons with fluorine in the C(12) Me group in the side chain and altering the orientation of the aryl groups around the double bond from anti to syn lowered ODC activity in both the thiochroman- and chroman-contg. systems. Esters VII and IX and acid VIII were essentially inactive while acid X exhibited a high ID₅₀ in the ODC assay. In the chroman family, both ester XI and acid XII had unfavorable ID₅₀ values. Since acid VIII differs only slightly from acid X [the latter is devoid of the geminal di-Me group at C(2)] and acid X differs only slightly from acid XII, possibly the nature of the heteroatom and the stereochem. at the .alpha. position may play important roles in regulating activity, but more examples are required to establish a trend. Changing the ring size from a fused six-six system to a five-six system led to ester Me (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]**benzoate** (XIII) and acid (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]**benzoic** acid (XIV),

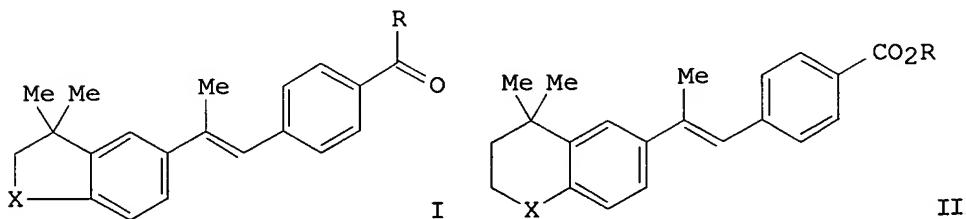
resp. In sep. expts. from those with of I-XII and known compds both XIII and XIV exhibited similar inhibition of ODC activity to that of III at the 34 nmol level. The ID50 values of XIV and XIV were, however, 10 and 200 times greater than that of III resp. In view of the toxicity of III, ester XIII may hold promise in chemotherapy. Of eight **heteroarotinoids** examd. in the HL-60 assay system, only acid IV displayed modest activity. This acid had an ED50 value (dose required for half-maximal effect) of 500 nM. In comparison, the ED50 for III was 50 nM. All of the other **heteroarotinoids** had ED50 values which were greater than 1000 nM.

L13 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids:** analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples
AN 1990:424286 CAPLUS
DN 113:24286
TI **Heteroarotinoids:** analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples
AU Gale, Jonathan B.; Rajadhyaksha, Shirish N.; Spruce, Lyle W.; Berlin, K. Darrell; Ji, Xinhua; Slagle, Andrew; Van der Helm, Dick
CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA
SO Journal of Organic Chemistry (1990), 55(13), 3984-91
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 113:24286
AB A series of derivs. of E and Z isomers of 4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzopyran-6-yl)-1-propenyl]benzoic acid and 4-[2-(2,3-dihydro-3,3-dimethyl-5-benzofuranyl)-1-propenyl]benzoic acid and sulfur-contg. counterparts were examd. in terms of 1H, 13C, and UV analyses for the purpose of establishing which parameters are diagnostic for identifying E and Z isomers in this family of **heteroarotinoids**. In addn., x-ray diffraction analyses for Me (E)-[2-(2,3-dihydro-3,3-dimethyl-5-benzofuranyl)-1-propenyl]benzoate (I), Me (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]benzoate (II), and Me (Z)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]benzoate (III) were performed to confirm the arrangement around the central double bond in the solid state in these rare examples contg. a fused, five-six-membered ring system. The proton NMR analyses of solns. of the E vs. the Z isomers, particularly the enhanced shielding of the vinylic proton and protons at "ortho" positions on the aryl groups attached to the double bond, provide markers to identify the Z isomers in these **heteroarotinoids**. In the 13C spectra, the Me C attached to the double bond was usually about 10 ppm downfield in the Z isomer compared to the counterpart in the E isomer. These data suggest that in soln. the two aryl rings in the Z isomers, (and possibly the E isomers, are turned out of the plane of the double bond, and, due to the closer proximity of the rings, induced shielding of nearby protons occurs to a greater extent in the Z isomers, compared to the E isomers. This evaluation is supported by UV spectral data which show max. in two ranges, namely at 210-270 and 280-350 nm. The "conjugation band" at the longer wavelength is always more intense, relative to the band at the shorter wavelength, in the E isomers. This implies improved overlap of p orbitals in the double bond with those in the aryl rings in the E isomers. In contrast, the band at shorter wavelength is more intense than the band at long wavelength in the Z isomers. These two features are clearly distinguishing for the two isomeric forms in soln. and relate to some degree to the stilbene isomerism. Characterization of I, II, and III via x-ray diffraction anal. of single crystals confirmed that the rings in both isomeric alkenes lack coplanarity with the central double bond in the solid state. The deviation from overall planarity is greatest for the Z

isomers with the internal torsional angle being 10.1.degree. in III rather than the "ideal" value of 0.degree.. Moreover, the aryl rings are not far from being nearly perpendicular to each other in III. Mol. mechanics calcns., using the MM2 program, indicate that the deviation from planarity is less than that found from x-ray anal. on solid III. These data provide a foundation for rapid identification of certain groups of heteroarotinoids. A comparison of crystal data of I and II with that of trans-retinoic acid was also made. The least-squares "fit" is quite satisfactory in spite of differences in conformational angles, and an RMS value of 0.90 .ANG. is calcd.

L13 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS
 TI Heteroarctinoid compounds as anticancer agents
 AN 1989:573986 CAPLUS
 DN 111:173986
 TI Heteroarctinoid compounds as anticancer agents
 IN Berlin, Kenneth D.; Holt, Elizabeth M.; Ford, Warren T.; Thompson, Mark D.
 PA Oklahoma State University, USA
 SO U.S., 18 pp. Cont.-in-part of U.S. Ser. No. 598,482, abandoned.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4826984	A	19890502	US 1987-9083 US 1984-598482	19870127 19840409
OS	CASREACT 111:173986; MARPAT 111:173986				
GI					

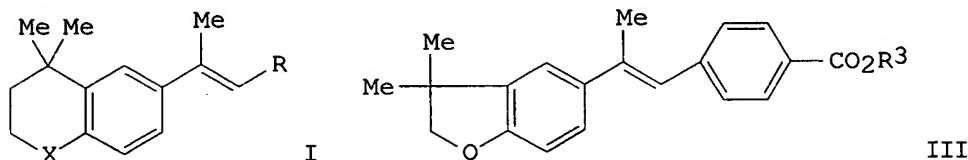


AB **Heteroarotinoids**, e.g., I ($R = H, OH, OMe, OEt$, etc.; $X = S, SO_2$), II ($R = H, Me, Et$; $X = O, S, SO$), etc., were prepd. as anticancer agents. Treatment of [1-(3,4-dihydro-4,4-dimethyl-2H-1-benzothiopyran-6-yl)ethyl]triphenylphosphonium bromide (prepn. given) with BuLi, followed by reaction with Et 4-formylbenzoate, gave, after workup, Et (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzothiopyran-6-yl)-1-propenyl]benzoate. In the HL-60 cell differentiation assay, (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzopyran-6-yl)-1-propenyl]benzoate exhibited an ED₅₀ of $> 3 \mu M$, vs. an ED₅₀ of 200 nM for tetrahydrotetramethylnaphthalenylpropenylbenzoic acid.

L13 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI **Heteroarotinoids.** Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells
AN 1987:576259 CAPLUS
DN 107:176259
TI **Heteroarotinoids.** Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the

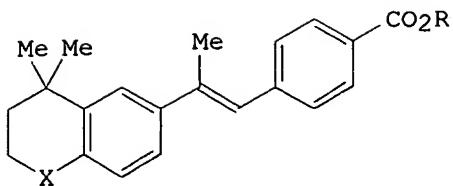
induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells

AU Spruce, Lyle W.; Rajadhyaksha, Shirish N.; Berlin, K. Darrell; Gale, Jonathan B.; Miranda, Edgar T.; Ford, Warren T.; Blossey, Erich C.; Verma, A. K.; Hossain, M. B.; et al.
CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA
SO Journal of Medicinal Chemistry (1987), 30(8), 1474-82
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 107:176259
GI

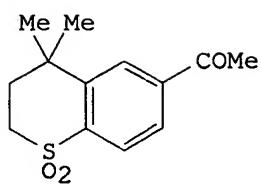


AB The heteroarotenoids I (X = S, R = CH:CHCMe:CHCO2R1, R1 = H, Et, 2-phthalimidoethyl) were prep'd. from 6-acetyl-4,4-dimethylthiochroman. I (X = O, R = CH:CHCMe:CHCO2H) was similarly obtained from 6-acetyl-4,4-dimethylchroman (II). I (X = O, R = 4-R2C6H4, R2 = CO2Me, CH2OH, cyano, CHO) were also obtained from II. **Benzofurans** III (R3 = Me, H) were prep'd. from 4-MeOC6H4Br and CH2:CMcCH2Cl. I (R = CH:CHCMe:CHCO2R1) showed high inhibition of ornithine decarboxylase, whereas I (R = 4-R2C6H4) and III were somewhat less active. In the HL-60 cell differentiation test I and III were substantially less active than trans-retinoic acid.

L13 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS
TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]benzoate.
AN 1985:24869 CAPLUS
DN 102:24869
TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]benzoate
AU Waugh, Kristy M.; Berlin, K. Darrell; Ford, Warren T.; Holt, Elizabeth M.; Carroll, John P.; Schomber, Paul R.; Thompson, M. Daniel; Schiff, Leonard J.
CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA
SO Journal of Medicinal Chemistry (1985), 28(1), 116-24
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
GI



I



III

AB **Heteroarotinoids I** [X, R = S, Et (II); O, Et; S(O), Et; O, H] and the dioxide III were prepd. and evaluated for their vitamin A activity. X-ray anal. data for II and III are given.

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BATCH **COMPLETE**
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PROJECTED ANSWERS: 0 TO 0

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FULL SCREEN SEARCH COMPLETED - 3132 TO ITERATE

100.0% PROCESSED 3132 ITERATIONS
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0 ANSWERS

L20 0 SEA SSS FUL L18

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FULL ESTIMATED COST	297.10	374.98
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION